

# LASER-INDUCED CONDUCTIVITY OF SEMICONDUCTORS AT LOW TEMPERATURES

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We consider the negative conductivity of electrons in semiconductors excited by a picosecond laser pulse at low temperatures, due to the inelastic electron–phonon collisions. For the first time, the dependence of the deformation potential on the phonon wave number is taken into account. This dependence significantly changes the region of negative electron conductivity as a function of the phonon temperature.

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## 1. INTRODUCTION

The possibility of the absolute negative conductivity of a small number of conducting electrons produced in some dielectrics and semiconductors by an external source was discussed previously [1, 2] (see also review [3]). In the case of diamond, the frequency of inelastic collisions with longitudinal acoustic phonons should increase near

$$m^* c^2/2 = 16 \text{ K},$$

where  $m^*$  is the electron effective mass and  $c$  is the speed of sound. If the electron speed is less than the speed of sound  $c$ , the phonon production is forbidden by the energy conservation law. It should be noted that in the case of Si, the quantity

$$m^* c^2/2 = 0.85 \text{ K}$$

is very small. Therefore, it is impossible in practice to observe the negative conductivity in Si, because the scattering of charge carriers on impurities resulting in positive conductivity dominates at very small temperatures. The absolute negative conductivity was observed experimentally only in gases [4]. For semiconductors, the negative mobility was observed for minor carriers due to their entrainment by the flow of major carriers in heterostructures [5] and for a two-dimensional electron gas in a strong external magnetic field. The goal of this

paper is a theoretical investigation of the conductivity and mobility in semiconductors at low temperatures irradiated by an ultra-short laser pulse.

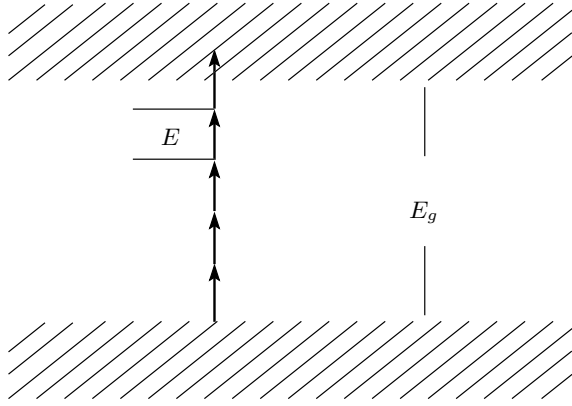
## 2. IONIZATION OF SEMICONDUCTORS BY THE FIELD OF AN INTENSE PICOSECOND LASER PULSE

We consider the production of carriers in semiconductors induced by an intense laser pulse with the pulse duration  $t \sim 1$  ps. It is well known that the threshold intensity for plasma production in most of the species at this pulse duration is of the order  $10^{11}$  W/cm<sup>2</sup> [6]. Hence, the total destruction of the crystal structure occurs at this laser intensity. We therefore suggest using the value of the peak laser intensity one order less, i.e.,  $I = 10^{10}$  W/cm<sup>2</sup>. In the case of a typical Nd:glass laser, the photon energy is equal to

$$E = \hbar\omega = 1.17 \text{ eV}.$$

We further consider the example of a diamond sample. For ionization of diamond with the band gap  $E_g = 5.4$  eV, the absorption of at least 5 photons is required (Fig. 1). Conducting electrons are produced with the initial energy about  $1.17 \cdot 5 - 5.4 = 0.45$  eV. The initial energy spectrum of conducting electrons is close to the Dirac delta-function distribution. This energy rapidly decreases close to the relaxation processes up to a value about tens K. The relaxation time with respect to the electron energy due to collisions of a

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**Fig. 1.** Scheme of photon absorption at the ionization of diamond

high-energy electron with acoustical phonons is well known [7, Eq. (8.23)],

$$\tau_r = \frac{2\pi\hbar^4\rho c^2}{(2m^*)^{3/2}T\Xi^2 E_p^{1/2}},$$

where  $\Xi$  is the deformation potential,  $T$  is the temperature of the crystal lattice,  $E_p$  is the electron kinetic energy,  $\rho$  is the mass density of a crystal,  $c$  is the speed of sound, and  $m^*$  is the effective mass of the carrier. The electron energy decreases to several hundreds of K during 100–1000 ps. About 100 collisions are needed for the total energy relaxation of an electron with the kinetic energy 100 K. This channel results in a large relaxation time due to quite elastic collisions of high-energy electrons with phonons.

The second channel for the relaxation is related to the production of the Wannier–Mott excitons with the binding energy

$$E_{ex} = E_g + \frac{p^2}{2(m_p^* + m_h^*)} - \frac{\mu e^4}{2\hbar^2 \varepsilon^2 n^2},$$

where  $n = 1, 2, 3, \dots$  is the principal quantum number,  $m_p^*$  and  $m_h^*$  are the respective effective masses of an electron and a hole,  $\mu$  is the reduced mass of the recombining electron and hole,  $\varepsilon$  is the dielectric constant of matter, and  $p$  is the exciton linear momentum. The radius of the exciton is large compared to the lattice constant. The decay of these excitons with emission of a spontaneous photon with the energy  $E_{ex} = cp$  occurs within 1–10 ps. Channels with additional emission or absorption of phonons are also possible.

Finally, an electron can recombine with a hole directly. The excess energy of this process (the so-called Auger recombination) is transferred to another con-

ducting electron. This channel is significant at a high number density of carriers.

In practice, recombination is mainly produced by impurities even at the negligibly small concentration of impurities. Conducting electrons and holes are captured by the levels of impurities.

We note that the Maxwell distribution of carriers is not established even during nanoseconds, because it is determined by electron–electron collisions and their collision frequency is small due to the small number density of conducting electrons.

The Keldysh parameter [8] is

$$\gamma_K = \frac{\omega\sqrt{2E_g}}{F} > 1$$

(atomic units are used, with the electron charge and effective mass and the Planck constant equal to unity) for the above values of the parameters. Here,  $\omega$  is the laser frequency. Thus, there is no tunneling ionization, but we have a 5-photon ionization process. The laser field strength is very small compared to the above-threshold field strength; therefore, there is no above-threshold ionization [9]. The peak laser field strength is  $F = 2.7 \cdot 10^6$  V/cm at the intensity  $10^{10}$  W/cm<sup>2</sup>. Of course, we must check that the diamond temperature does not exceed 600 °C in air and 1800 °C in a vacuum. This is just realized at the short laser pulse durations of the order of 1 ps.

We now consider the value of the generalized cross section for the 5-photon ionization. It is determined mainly by the ionization potential of the considered matter. There is no such data for diamond and other semiconductors, and we therefore used the known data [9] for Na atoms (the ionization potential is equal to 5.14 eV) and Ba atoms (the ionization potential is equal to 5.21 eV). According to the experimental data in [9], the generalized cross section is

$$\sigma_5 \approx 10^{-140} \text{ cm}^{10} \cdot \text{s}^4.$$

The cross section for  $K$ -photon ionization is related to the corresponding ionization rate as

$$w^{(K)} = \frac{\sigma_K I^K}{(\hbar\omega)^K},$$

where  $I$  is the peak laser intensity. With the above value of the laser peak intensity, we obtain

$$w^{(5)} \approx 4000 \text{ s}^{-1}.$$

Hence, the fraction of atoms ionized during the pulse duration is

$$w^{(5)}\tau \approx 4 \cdot 10^{-9}.$$

The values of the mass density  $\rho$  and the number density of atoms  $n$  in diamond are well known:

$$\rho = 3.51 \text{ g/cm}^3, \quad n = 1.75 \cdot 10^{23} \text{ cm}^{-3}.$$

Hence, the number density of conducting electrons and holes after the ionization process is

$$n_e = 7 \cdot 10^{14} \text{ cm}^{-3}.$$

At the normal incidence of a linearly polarized laser pulse to the surface of diamond, the field inside the matter is equal to the field in the vacuum. But at the oblique incidence of a linearly polarized laser beam to the diamond surface, the laser field inside the matter decreases due to a sufficiently large value of the dielectric constant of diamond,  $\varepsilon = 5.7$ . Hence, at the oblique incidence, the number of conducting electrons is less than the above value.

Diamond is an anisotropic matter, with the electron effective mass given by

$$m_{\parallel}^* = 1.50m_e$$

along the (100) direction [10] and

$$m_{\perp}^* = 0.26m_e$$

along the (010) direction ( $m_e$  is the vacuum electron mass). Therefore, the ionization depends on the types of charge carriers. We discuss the dependence of the generalized cross section for multiphoton ionization on the effective mass of the carrier. The dipole matrix element for the 5-photon transition is given by [11]

$$z_{mn}^{(5)} = \sum_{l,p,s,t} \frac{z_{ml}z_{lp}z_{ps}z_{st}z_{tn}}{(E_{lm}-\omega)(E_{pm}-2\omega)(E_{sm}-3\omega)(E_{tm}-4\omega)},$$

where  $z_{ml}$  is the usual dipole matrix element for the transition between atomic states  $m$  and  $l$ , and  $E_{lm}$  are differences of energies between these states. The dependence of the dipole matrix element on the effective mass and on the energy gap can be estimated in the hydrogen-like approximation as

$$z_{lm} \propto a \propto \frac{\pi\hbar}{\sqrt{2m^*E_g}},$$

where  $a$  is the corresponding effective Bohr radius. Thus, the dependence of the 5-photon ionization rate on the effective mass is

$$w^{(5)} \propto |z_{lm}|^2 \propto \frac{1}{(m^*)^5}.$$

It is seen that the 5-photon ionization rate increases sharply with decreasing the effective electron (or hole) mass. Thus, ionization is produced mainly in (010) direction of the diamond crystal. For this reason, the ionization rate of a diamond sample is larger than that of Na and Ba atoms by one to two orders of magnitude at the same value of laser intensity.

### 3. THE DEFORMATION POTENTIAL

Due to thermal motion of atoms in a crystal lattice, each element of the crystal volume is shifted by a small value  $\mathbf{u}(\mathbf{r}, t)$  with respect to its unshifted position  $\mathbf{r}$ . In the harmonic approximation, this shift can be expressed via the operators  $a_{\mathbf{k}}^+$  and  $a_{\mathbf{k}}$  of production and destruction of a longitudinal acoustic phonon (which is an independent oscillation of the lattice) as

$$\mathbf{u}(\mathbf{r}, t) = \frac{1}{\sqrt{2MN}} \times \sum_{\mathbf{k}} \frac{1}{\sqrt{\omega_{\mathbf{k}}}} \mathbf{e}_{\mathbf{k}} \{ a_{\mathbf{k}} \exp [i(\mathbf{k} \cdot \mathbf{r} - \omega_{\mathbf{k}}t)] + a_{\mathbf{k}}^+ \exp [-i(\mathbf{k} \cdot \mathbf{r} - \omega_{\mathbf{k}}t)] \}, \quad (1)$$

where  $N$  is the number of atoms in the crystal sample,  $M$  is the mass of the atom,  $\mathbf{e}_{\mathbf{k}}$  is the unit polarization vector for the longitudinal phonon, i.e., the unit vector along the phonon wave vector  $\mathbf{k}$  (we see in what follows that the transverse acoustic phonons do not contribute to the crystal conductivity), and  $\omega_{\mathbf{k}}$  is the phonon frequency, which is related to the wave number  $\mathbf{k}$  (in the approximation of small wave numbers, i.e., large wavelengths in comparison with the lattice constant) as

$$\omega_{\mathbf{k}} = ck, \quad (2)$$

with  $c$  being the longitudinal speed of sound. The upper limit of the acoustic oscillations corresponds to the lattice temperature about 100–300 K.

The small perturbation of the potential for a conducting electron produced by surrounding atoms in the crystal lattice because of the lattice deformation is

$$U(\mathbf{r}) = V(\mathbf{r}) - V(\mathbf{r} + \mathbf{u}) \approx -\mathbf{u} \cdot \nabla V. \quad (3)$$

The conducting electron wave function is the Bloch function normalized by the number of these electrons  $N$ :

$$\psi_{\mathbf{p}}(\mathbf{r}, t) = \frac{1}{\sqrt{N}} \varphi_{\mathbf{p}}(\mathbf{r}) \exp [i(\mathbf{p} \cdot \mathbf{n} - E_{\mathbf{p}}t)], \quad (4)$$

where  $p$  is the electron momentum,  $E_{\mathbf{p}}$  is its energy,  $\varphi_{\mathbf{p}}(\mathbf{r})$  is the periodic function with the period of the

lattice, and  $\mathbf{n}$  is the coordinate of a node of the crystal lattice. We note that because the number density of conducting electrons is small, we neglect the interaction between the produced conducting electrons and the screening effects.

In the first order of the quantum mechanical perturbation theory in interaction (3), the electron transition amplitude from the state with a momentum  $\mathbf{p}$  to a state with a momentum  $\mathbf{p}'$  due to the lattice deformation is

$$i \frac{dC(\mathbf{p}', t)}{dt} = \int \psi_{\mathbf{p}'}^*(\mathbf{r}, t) U(\mathbf{r}, t) \psi_{\mathbf{p}}(\mathbf{r}, t) d\mathbf{r}. \quad (5)$$

The matrix elements of the phonon operators of a harmonic oscillator are well known:

$$\begin{aligned} \langle N_{\mathbf{k}} - 1 | a_{\mathbf{k}} | N_{\mathbf{k}} \rangle &= \sqrt{N_{\mathbf{k}}}, \\ \langle N_{\mathbf{k}} + 1 | a_{\mathbf{k}}^\dagger | N_{\mathbf{k}} \rangle &= \sqrt{N_{\mathbf{k}} + 1}, \end{aligned} \quad (6)$$

where  $N_{\mathbf{k}}$  is the number of acoustic longitudinal phonons with the wave vector  $\mathbf{k}$ .

Substituting Eq. (4) in Eq. (5), we obtain that the integral in Eq. (5) factors into the product of an integral over one lattice cell and a sum over all nodes of the crystal lattice. This sum is of the form

$$\begin{aligned} \sum_{\mathbf{n}} \exp [i(\mathbf{p} - \mathbf{p}' \pm \mathbf{k}) \cdot \mathbf{n}] &= N, \\ \mathbf{p}' &= \mathbf{p} \pm \mathbf{k}. \end{aligned} \quad (7)$$

We thus obtain the momentum conservation law, Eq. (7), at the absorption or emission of a phonon of the crystal lattice by an electron.

The integration over one lattice cell in Eq. (5) can be carried out by parts,

$$\begin{aligned} I &= -\mathbf{e}_{\mathbf{k}} \int \varphi_{\mathbf{p}'}^* \varphi_{\mathbf{p}} \nabla V d\mathbf{r} = - \int \varphi_{\mathbf{p}'}^* \varphi_{\mathbf{p}} \frac{\partial V}{\partial \mathbf{s}} d\mathbf{r} = \\ &= \int V \frac{\partial}{\partial \mathbf{s}} (\varphi_{\mathbf{p}'}^* \varphi_{\mathbf{p}}) d\mathbf{r}, \end{aligned} \quad (8)$$

where the coordinate  $\mathbf{s}$  corresponds to the direction of the polarization vector  $\mathbf{e}_{\mathbf{k}}$ . To calculate the integral in Eq. (8), we consider the Schrödinger equation for a conducting electron in the potential  $V$  of surrounding atoms:

$$\Delta \psi_{\mathbf{p}} + 2(E_{\mathbf{p}} - V) \psi_{\mathbf{p}} = 0. \quad (9)$$

The electron effective mass is here set equal to unity. Substituting Eq. (4) in Eq. (9), we rewrite this equation as

$$\Delta \varphi_{\mathbf{p}} + 2i(\mathbf{p} \cdot \nabla \varphi_{\mathbf{p}}) - p^2 \varphi_{\mathbf{p}} + 2(E_{\mathbf{p}} - V) \varphi_{\mathbf{p}} = 0. \quad (10)$$

Using the conjugate expression in which we substitute  $\mathbf{p} \rightarrow \mathbf{p}'$ , we obtain

$$\Delta \varphi_{\mathbf{p}'}^* - 2i(\mathbf{p}' \cdot \nabla \varphi_{\mathbf{p}'}^*) - p'^2 \varphi_{\mathbf{p}'}^* + 2(E_{\mathbf{p}'} - V) \varphi_{\mathbf{p}'}^* = 0. \quad (11)$$

Multiplying Eq. (10) by  $\partial \varphi_{\mathbf{p}'}^* / \partial \mathbf{s}$  and Eq. (11) by  $\partial \varphi_{\mathbf{p}} / \partial \mathbf{s}$ , we add both equations and then integrate the sum over  $\mathbf{r}$ , simultaneously using integration by parts:

$$\begin{aligned} i(\mathbf{p} - \mathbf{p}') \int \frac{\partial \varphi_{\mathbf{p}'}^*}{\partial \mathbf{s}} \nabla \varphi_{\mathbf{p}} d\mathbf{r} + \left( E_{\mathbf{p}} - E_{\mathbf{p}'} - \frac{p^2}{2} + \frac{p'^2}{2} \right) \times \\ \times \int \frac{\partial \varphi_{\mathbf{p}'}^*}{\partial \mathbf{s}} \varphi_{\mathbf{p}} d\mathbf{r} - \int V \frac{\partial}{\partial \mathbf{s}} (\varphi_{\mathbf{p}'}^* \varphi_{\mathbf{p}}) d\mathbf{r} = 0. \end{aligned} \quad (12)$$

The second term in this expression can be neglected compared to the first term, because their ratio is of the order of the electron momentum  $p$  times the lattice constant  $a$ . This product is small compared to unity because of the small population of the conduction band by electrons at ionization.

Then, substituting Eq. (12) in Eq. (8), we obtain

$$\begin{aligned} I &= i(\mathbf{p} - \mathbf{p}') \int \frac{\partial \varphi_{\mathbf{p}'}^*}{\partial \mathbf{s}} \nabla \varphi_{\mathbf{p}} d\mathbf{r} = \mp i \mathbf{k} \int \frac{\partial \varphi_{\mathbf{p}'}^*}{\partial \mathbf{s}} \nabla \varphi_{\mathbf{p}} d\mathbf{r} = \\ &= \mp i \int (\mathbf{e}_{\mathbf{k}} \nabla \varphi_{\mathbf{p}'}^*) (\mathbf{k} \cdot \nabla \varphi_{\mathbf{p}}) d\mathbf{r}. \end{aligned} \quad (13)$$

Because the longitudinal phonon vectors  $\mathbf{k}$  and  $\mathbf{e}_{\mathbf{k}}$  have the same direction, integration over the angular variables of  $\mathbf{r}$  can be carried out directly. With the angle between the polarization vector of the phonon and the vector  $\mathbf{r}$  denoted by  $\chi$ , we find

$$\langle \cos^2 \chi \rangle = 1/3$$

after the averaging. Moreover, an analogous averaging procedure for both transverse phonons gives zero. Thus, only the interaction with longitudinal phonons is significant in the considered problem (we have already made this assumption above). It follows from Eq. (13) that

$$\begin{aligned} I &= \mp \frac{i}{3} k \int (\nabla \varphi_{\mathbf{p}'}^* \cdot \nabla \varphi_{\mathbf{p}}) d\mathbf{r} \approx \\ &\approx \mp \frac{i}{3} k \int |\nabla \varphi_{\mathbf{p}}|^2 d\mathbf{r} = \mp i k \Xi, \\ \Xi &= \frac{1}{3} \int |\nabla \varphi_{\mathbf{p}}|^2 d\mathbf{r}. \end{aligned} \quad (14)$$

According to experimental data, it depends slowly on the electron momentum  $p$ . From the theoretical standpoint, this slow dependence is the strong-coupling approximation for conducting electrons. This approximation is valid when the kinetic energy of the conducting electron is less than the lattice temperature. We neglect the overlap of the electron wave functions in different crystal cells.

The deformation potential is determined by the change in the deformation energy of a crystal at the

variation of its volume. Fitting the experimental data on mobility of electrons and holes at the temperatures in the range 100–1000 K allows finding the values of the deformation potential; these data confirm its weak dependence on the carrier energy.

The ground-state Hartree–Fock wave function of the carbon atom is a product of single-particle wave functions of four valence electrons, in  $2s$  states (two electrons) and  $2p$  states (two filled and four empty sub-states). In a crystal, this level spreads into a band filled by electrons. During the dipole transition at the ionization, an electron is transferred from the  $2s$  to  $2p$  state. In a crystal, this excited state spreads into a band that is partially filled with conducting electrons. These electrons can tunnel from one crystal cell to another. The lattice constant for diamond is  $a = 0.36$  nm, and therefore  $pa \ll \hbar$  even at the initial electron energy 0.45 eV. Hence, most of the conducting electrons are placed near the center of the Brillouin zone, and the parabolic approximation is valid for their energies. Also, the electron–phonon scattering resulting in the transitions of an electron to the neighboring Brillouin zones can be neglected.

We also substituted  $\mathbf{p}' \rightarrow \mathbf{p}$  in Eq. (14). The underlying assumption is very strong. At high temperatures, when the electron speed is large in comparison with the speed of sound  $c$ , the phonon energy is small compared to the electron energy; therefore, electron energies before and after the phonon absorption or emission are approximately equal to each other. Then the above assumption is valid. But if the electron speed is about of the speed of sound (inelastic processes), then this approximation is incorrect.

The quantity

$$\frac{1}{2} \int |\nabla \varphi_{\mathbf{p}}|^2 d\mathbf{r} \quad (15)$$

is the average kinetic energy of a conducting electron inside the crystal cell [12]. Of course, it is not equal to

$$E_p = p^2/2m^*,$$

because the electron wave function is similar to the plane wave only for almost free electrons, whereas we here have the opposite case of strong-coupled electrons. Just the exponent in the Bloch function, Eq. (4), is responsible for the kinetic energy  $p^2/2m^*$  which is a small part of the quantity in Eq. (15).

In the case of small values of  $p'$ , it follows from the Taylor expansion that

$$|\nabla \varphi_{\mathbf{p}'}| \sim p'. \quad (16)$$

The final new expression for the quantity  $I$  follows from Eqs. (13) and (16) as

$$I = \mp ik \Xi \frac{p'}{p}. \quad (17)$$

Because  $p' < p$ , the variable deformation potential is less than the constant deformation potential that is used in typical calculations of the kinetics of carriers in semiconductors. Of course, at high electron energies (more than 1000 K), we have  $p' = p$ .

#### 4. TRANSPORT COLLISION FREQUENCY

Substituting Eq. (17) in Eq. (5) and taking Eq. (6) into account, we obtain the transition amplitudes

$$\begin{aligned} \frac{dC(\mathbf{p} + \mathbf{k}, t)}{dt} &= -\Xi \frac{k}{p} p' \sqrt{\frac{N_{\mathbf{k}}}{2MN\omega_{\mathbf{k}}}} \times \\ &\times \exp[i(E_{\mathbf{p}+\mathbf{k}} - E_{\mathbf{p}} - \omega_{\mathbf{k}})t], \\ \frac{dC(\mathbf{p} - \mathbf{k}, t)}{dt} &= \Xi \frac{k}{p} p' \sqrt{\frac{N_{\mathbf{k}} + 1}{2MN\omega_{\mathbf{k}}}} \times \\ &\times \exp[i(E_{\mathbf{p}+\mathbf{k}} - E_{\mathbf{p}} + \omega_{\mathbf{k}})t]. \end{aligned} \quad (18)$$

After the integration of temporal exponentials, we find

$$\begin{aligned} J &= \int_0^t \exp[i(E_{\mathbf{p}+\mathbf{k}} - E_{\mathbf{p}} \pm \omega_{\mathbf{k}})t] dt = \\ &= \frac{\exp[i(E_{\mathbf{p}+\mathbf{k}} - E_{\mathbf{p}} \pm \omega_{\mathbf{k}})t] - 1}{i(E_{\mathbf{p}+\mathbf{k}} - E_{\mathbf{p}} \pm \omega_{\mathbf{k}})}, \\ |J|^2 &= 2\pi t \delta(E_{\mathbf{p}+\mathbf{k}} - E_{\mathbf{p}} \pm \omega_{\mathbf{k}}). \end{aligned} \quad (19)$$

The Dirac delta-function demonstrates the energy conservation law at the absorption or emission of a phonon by an electron. It follows from Eqs. (18) and (19) that

$$\begin{aligned} |C(\mathbf{p} + \mathbf{k}, t)|^2 &= \\ &= \Xi^2 \frac{\pi N_{\mathbf{k}} k^2 p'^2}{MN\omega_{\mathbf{k}} p^2} t \delta(E_{\mathbf{p}+\mathbf{k}} - E_{\mathbf{p}} - \omega_{\mathbf{k}}), \\ |C(\mathbf{p} - \mathbf{k}, t)|^2 &= \\ &= \Xi^2 \frac{\pi (N_{\mathbf{k}} + 1) k^2 p'^2}{MN\omega_{\mathbf{k}} p^2} t \delta(E_{\mathbf{p}+\mathbf{k}} - E_{\mathbf{p}} + \omega_{\mathbf{k}}), \end{aligned} \quad (20)$$

where the equilibrium population number of phonons is given by the Bose distribution

$$N_{\mathbf{k}} = \frac{1}{\exp(\omega_{\mathbf{k}}/T) - 1} \quad (21)$$

with  $T$  being the phonon (lattice) temperature (measured in energy units).

Equation (20) can be rewritten in the form that fixes the final electron momentum  $\mathbf{p}'$  and determines the transition rate:

$$w_{\mathbf{p}\mathbf{p}'} = \frac{|C(\mathbf{p}', t)|^2}{t} = \Xi^2 \frac{\pi k^2 p^2}{MN\omega_{\mathbf{k}p'^2}} \times \\ \times \{N_{\mathbf{k}}\delta(E_{\mathbf{p}'} - E_{\mathbf{p}'-\mathbf{k}} - \omega_{\mathbf{k}}) + \\ + (N_{\mathbf{k}} + 1)\delta(E_{\mathbf{p}'} - E_{\mathbf{p}'+\mathbf{k}} + \omega_{\mathbf{k}})\}. \quad (22)$$

This expression allows us to derive the collision frequency between electrons and phonons after integration over angles; we multiply Eq. (22) by  $V d\mathbf{k}/(2\pi)^3$  (where  $V$  is the volume of the sample) and integrate over the phonon wave vector. To obtain the transport collision frequency, we additionally multiply Eq. (22) by the factor  $(p - p' \cos \theta)/p$ , where  $\theta$  is the scattering angle (the angle between the vectors  $\mathbf{p}$  and  $\mathbf{p}'$ ):

$$\nu_{ph} = \int w_{\mathbf{p}\mathbf{p}'} \frac{p - p' \cos \theta}{p} \frac{V d\mathbf{k}}{(2\pi)^3}. \quad (23)$$

Integrating over the angle  $\vartheta$  between the vectors  $\mathbf{k}$  and  $\mathbf{p}$  and taking the relation

$$p - p' \cos \theta = \pm k \cos \vartheta \quad (24)$$

into account gives the transport collision frequency as

$$\nu_{ph} = \Xi^2 \frac{m^*}{4\pi\rho c\hbar^2 p^3} \left( \int_0^{\max(0; 2p-2m^*c/\hbar)} (N_{\mathbf{k}} + 1) \times \right. \\ \times \left( 1 - \frac{2m^*ck}{\hbar p^2} \right) \left( \frac{m^*ck}{\hbar} + \frac{k^2}{2} \right) k^2 dk - \\ - \int_{\max(0; 2m^*c/\hbar-2p)}^{2m^*c/\hbar+2p} N_{\mathbf{k}} \left( 1 + \frac{2m^*ck}{\hbar p^2} \right) \times \\ \left. \times \left( \frac{m^*ck}{\hbar} - \frac{k^2}{2} \right) k^2 dk \right). \quad (25)$$

We here restored the Planck constant;  $\rho$  is the mass density of matter. Knowing the collision frequency, we can derive the electron mobility  $b$ . For this, we assume 1) the validity of the relaxation-time approximation, 2) the delta-functional distribution of the carriers (single-energy approximation), and 3) the cubic shape of the crystal. Finally, we can write

$$b(\varepsilon, T) = \frac{1}{m^*\nu_{ph}} + \frac{2\varepsilon_p}{3m^*} \frac{d}{d\varepsilon_p} \left( \frac{1}{\nu_{ph}} \right), \quad (26)$$

where  $\varepsilon_p = p^2/2m^*$  is the electron energy and  $m^*$  is the electron (or hole) effective mass.

We must also take the elastic scattering of electrons on the acceptor impurities into account (mainly boron acceptor centers in the case of diamond with the ionization potential 0.37 eV). Then the frequency  $\nu_{ph}$  is to be replaced in Eq. (26) with the sum

$$\nu_t = \nu_{ph} + \nu_{imp},$$

where the frequency of collisions of electrons with impurities is given by the simple expression

$$\nu_{imp} = n_{imp} \sigma_{imp} \sqrt{\frac{2\varepsilon_p}{m^*}}. \quad (27)$$

Here,  $\sigma_{imp}$  is the cross section for scattering of electrons on impurities and  $n_{imp}$  is the boron impurity number density. In calculations, we use the values  $\sigma_{imp} = 10^{-14} \text{ cm}^2$  and  $n_{imp} = 10^{17} \text{ cm}^{-3}$ .

Finally, the electric conductivity  $\gamma$  can be related to the mobility  $b$  as

$$\gamma = n_e |e| b, \quad (28)$$

where  $n_e$  is the number density of carriers.

## 5. RESULTS

The speed of sound in diamond is  $c = 18.6 \text{ km/s}$ . The phonon temperature is chosen as  $T = 1, 10, 25,$  and  $100 \text{ K}$ . The effective electron longitudinal mass is  $m^* = 1.5m_e$ , and the effective light hole mass is  $m^* = 0.7m_e$  [10].

The constants of the deformation potential were chosen as  $\Xi = 11.5 \text{ eV}$  for holes and  $\Xi = 4.1 \text{ eV}$  for electrons. We obtained these constants from the experimental dependence  $b(T)$  in [13, 14] by fitting it with the dependence

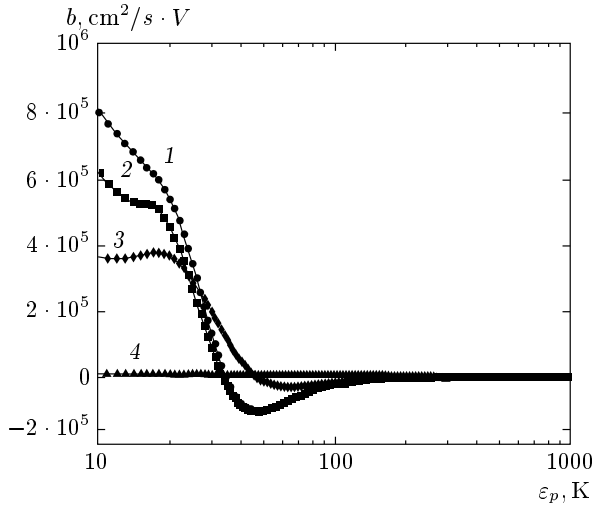
$$b(T) = \frac{2}{3T} \frac{\int_0^\infty (1/\nu_t(\varepsilon)) \varepsilon^{3/2} \exp(-\varepsilon/T) d\varepsilon}{\int_0^\infty \varepsilon^{1/2} \exp(-\varepsilon/T) d\varepsilon}.$$

In the range of lattice temperatures from 100 to 1000 K, this dependence can be simplified:

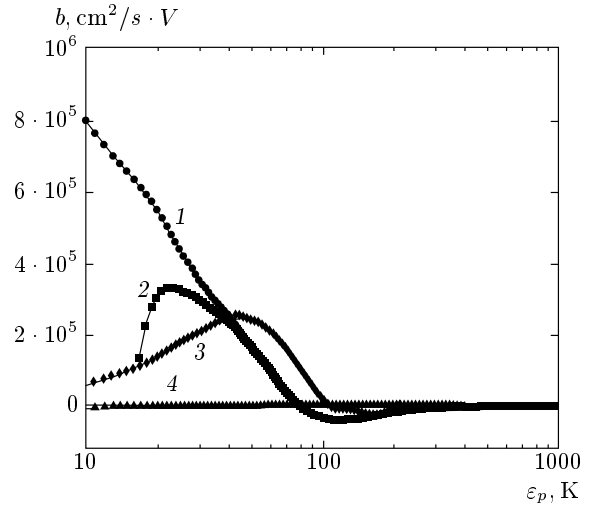
$$b(T) = \frac{\text{const}}{T^\alpha},$$

where  $\alpha = 1.5$  for electrons and  $\alpha = 3$  for holes.

Computations were made both with the dependence of the deformation potential on the phonon wave number  $\mathbf{k}$  taken into account and in the approximation of a



**Fig. 2.** The electron mobility in diamond as a function of the electron kinetic energy at various values of the phonon temperature  $T = 1$  (1), 10 (2), 25 (3), 100 (4) K. The case of a constant deformation potential

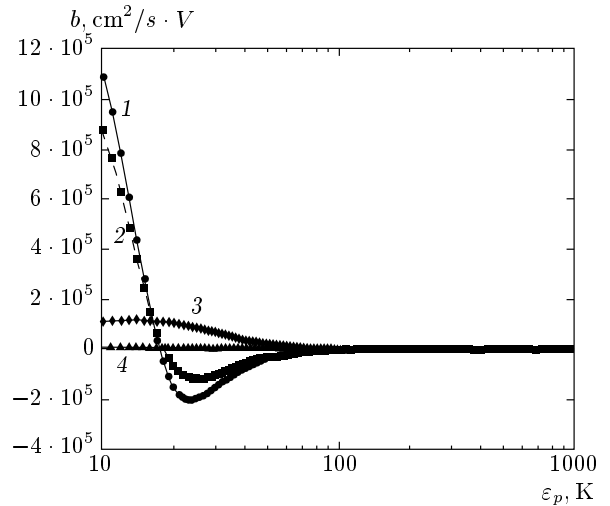


**Fig. 3.** The electron mobility in diamond as a function of the electron kinetic energy at various values of the phonon temperature  $T = 1$  (1), 10 (2), 25 (3), 100 (4) K. The case of a variable deformation potential

constant deformation potential; the latter can be found in Ref. [13]. In the case of a constant deformation potential, instead of Eq. (25), we find the electron–phonon collision frequency in the known form

$$\nu_{ph} = \Xi^2 \frac{m^*}{4\pi\rho c\hbar^2 p^3} \left( \int_0^{\max(0; 2p - 2m^*c/\hbar)} (N_k + 1) \times \left( \frac{m^*ck}{\hbar} + \frac{k^2}{2} \right) k^2 dk - \int_{\max(0; 2m^*c/\hbar - 2p)}^{2m^*c/\hbar + 2p} N_k \left( \frac{m^*ck}{\hbar} - \frac{k^2}{2} \right) k^2 dk \right). \quad (29)$$

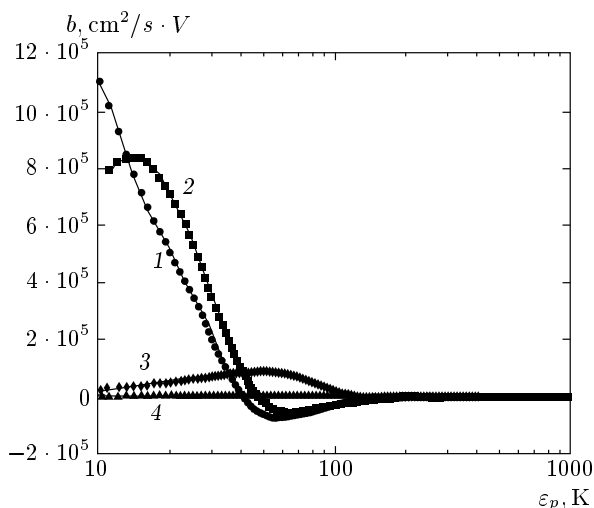
The results of computations are presented in Figs. 2 and 3. It can be seen from these figures that the dependence of the deformation potential on the phonon wave number shifts the negative electron mobility region to larger electron energies and reduces the value of the mobility in this region. For example, at the lattice temperature  $T = 10$  K, the range of negative conductivity and mobility is realized for electron energies between 60 and 200 K (Fig. 3). In the case of a constant deformation potential (Fig. 2), this interval is shifted to 20–100 K. We also show analogous results for holes in diamond (Figs. 4 and 5). The role of acceptor impurities is significant at very low temperatures, where they of course produce positive mobility, which is much larger than



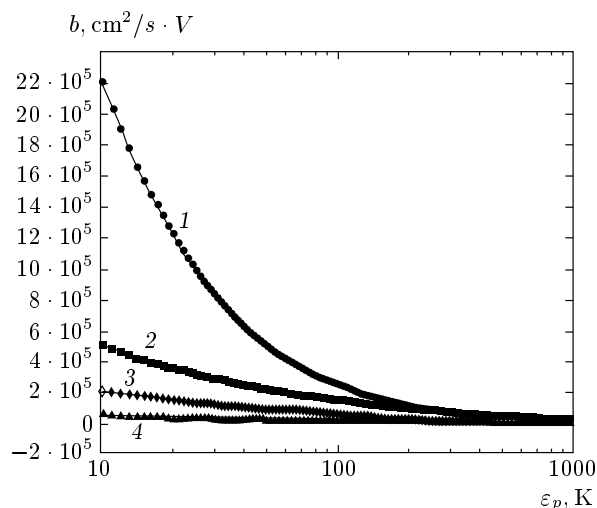
**Fig. 4.** The hole mobility in diamond as a function of the electron kinetic energy at various values of the phonon temperature  $T = 1$  (1), 10 (2), 25 (3), 100 (4) K. The case of a constant deformation potential

the negative contribution from electron–phonon inelastic collisions.

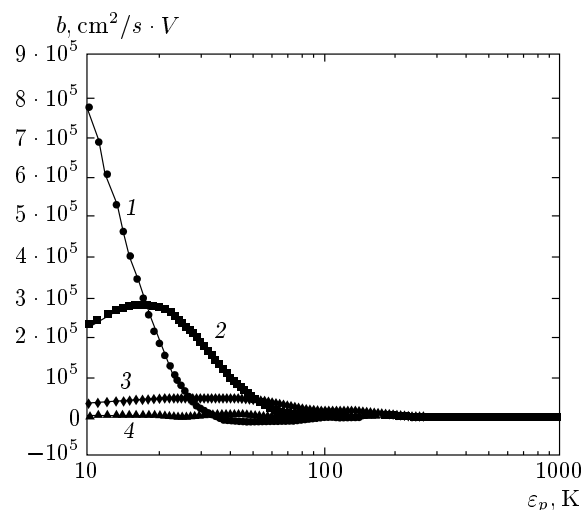
In Fig. 6, the mobility of holes in Si is presented as a function of the electron temperature for a variable deformation potential. It is seen that the negative-mobility region occurs only at the lattice temperature 1 K and is small. This is explained by the small speed



**Fig. 5.** The hole mobility in diamond as a function of the electron kinetic energy at various values of the phonon temperature  $T = 1$  (1),  $10$  (2),  $25$  (3),  $100$  (4) K. The case of a variable deformation potential



**Fig. 7.** The hole mobility in Ge as a function of the electron kinetic energy at various values of the phonon temperature  $T = 1$  (1),  $10$  (2),  $25$  (3),  $100$  (4) K. The case of a variable deformation potential



**Fig. 6.** The electron mobility in Si as a function of the electron kinetic energy at various values of the phonon temperature  $T = 1$  (1),  $10$  (2),  $25$  (3),  $100$  (4) K. The case of a variable deformation potential

of sound in Si ( $9.35 \text{ km/s}$ ). The electron mobility in Ge is shown in Fig. 7. It is positive for all values of the parameters (the speed of sound in Ge is  $5.56 \text{ km/s}$ ). Scattering of carriers on impurities determines the mobility. The electron–phonon interaction is negligibly small in this case.

The energy spectrum of electrons and holes is broadening during their relaxation. Describing this process requires solving the kinetic equation. But the

qualitative conclusion about negative conductivity at low electron energies remains correct.

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### СПИСОК ЛИТЕРАТУРЫ

1. В. Ф. Елесин, Е. А. Маныкин, Письма в ЖЭТФ **3**, 26 (1966).
2. В. Ф. Елесин, Е. А. Маныкин, ЖЭТФ **23**, 1381 (1966).
3. A. C. Durst and S. H. Girvin, Science **304**, 1762 (2004).
4. J. M. Warman, U. Sowada, and M. P. De Haas, Phys. Rev. A **31**, 1974 (1985).
5. R. A. Höpfel, J. Shah, P. A. Wolff, and A. C. Gossard, Phys. Rev. B **37**, 6941 (1988).
6. A. P. Matafonov, private communication.
7. R. A. Smith, *Semiconductors*, Cambridge University Press, Cambridge (1978).
8. Л. В. Келдыш, ЖЭТФ **20**, 1307 (1965).



9. N. B. Delone and V. P. Krainov, *Multiphoton Processes in Atoms*, Springer Verlag, Berlin (2000).
10. M. Willatzen, M. Cardona, and N. E. Christensen, *Phys. Rev. B* **50**, 24 (1994).
11. M. Ammosov, I. Bondar, N. Delone, M. Ivanov, and A. Masalov, *Adv. At. Mol. Phys.* **27**, 34 (1991).
12. P. Y. Yu and M. Cardona, *Fundamentals of Semiconductors*, Springer (2002).
13. A. S. Baturin, V. N. Gorelkin, V. S. Rastunkov, and V. N. Soloviev, *Physica B* **374-375**, 340 (2006).
14. А. П. Бабичев, Н. А. Бабушкина, А. М. Братковский и др., в кн. *Физические величины. Справочник*, под ред. И. С. Григорьева, Е. З. Мельникова, Энергоатомиздат, Москва (1991), с. 458.