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Constants of Electron-Phonon Interaction for Optical and Intervalley Phonons in *n*-Ge

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The electron scattering in the case of four-valley, two-valley and single-valley L_1-models of the conduction band of germanium single-crystals is investigated. The constants of electron-phonon interaction for optical $\Xi_{430} = 4 \cdot 10^8$ eV/cm and intervalley $\Xi_{320} = 1.4 \cdot 10^8$ eV/cm phonons in *n*-Ge on the base of the theory of anisotropic scattering and experimentally obtained temperature dependences of the resistivity are derived. It is shown that except of the electron scattering by acoustic phonons and impurity ions, electron scattering by optical and intervalley phonons should be taken into account in the four-valley L_1-model of the conduction band of *n*-Ge. Electron scattering by acoustic phonons is dominant in two- and single-valley L_1-model.

Keywords: Intravalley and intervalley scattering, Constant of electron-phonon interaction, Ellipsoid of revolution, Effective mass tensor, L_1 model of the conduction band of germanium crystal.

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1. INTRODUCTION

Germanium has always been and remains one of the key materials of modern semiconductor technology. It is used for the production of diodes, triodes, crystal detectors and power rectifiers. Single-crystal germanium is also used in dosimeters and devices which measure the strength of constant and alternating magnetic fields, in the infrared technology for the production of infrared detectors operating in the range of 8-14 μm, picosecond optoacoustics [1, 2]. Modern investigations in the field of nanotechnology show that germanium is also a promising material for nanoelectronics needs. Thus, use of nanostructures with self-induced Ge/Si nanoislands opens new prospects for the development of opto- and nanoelectronics [3]. Arrays of Ge (GeSi) quantum dots can be successfully applied for manufacturing photodetectors for near infrared range and light emitting diodes of the same spectral region [4]. Design on the basis of germanium of the mentioned electronic devices with the desired characteristics requires knowledge of the parameters of the material energy-band structure, scattering mechanisms of charge carriers, investigation of various kinetic and optical effects. Simple theory of electron scattering in *n*-Ge and *n*-Si gives the power law $\mu \sim T^{3/2}$ that corresponds to the scattering by acoustic phonons. But this law, as a rule, is not experimentally fulfilled in *n*-Ge, and, especially, in *n*-Si. The disagreement between theory and experiment is explained by additional mechanisms of electron scattering by optical and intervalley phonons. Interaction between electrons and intervalley phonons plays an important role for the nondirect band optical transitions connected with hot electrons [5], influences the low-frequency fluctuations of electric current [6]. At present, intervalley scattering in *n*-Si, in contrast to *n*-Ge, is well studied, since it is already rather effective at temperatures of $T > 100$ K [7].

Electron-phonon interaction constants are the main parameters which characterize electron scattering by optical and intervalley phonons. Currently, there is very few information about these parameters in *n*-Ge in the literature. At that, theoretical calculations using electron-phonon interaction constants determined by certain method, as a rule, do not always agree with the experimental results of unrelated investigations, and, therefore, require constant corrections [8].

2. RESULTS OF THE EXPERIMENTAL INVESTIGATIONS

To study the features of electron-phonon interaction in *n*-Ge we have studied electron scattering in four-, two-, and single-valley L_1-model of the conduction band of germanium single-crystals. For unstrained *n*-Ge single-crystals, conduction band will consist of four constant-energy surfaces which are ellipsoids of revolution [9]. Two- and single-valley L_1-models in a wide temperature range can be obtained at strong uniaxial pressure $P \sim 1.8$ GPa along the crystallographic directions [110] and [111], respectively [10]. In Fig. 1-Fig. 3 we present the temperature dependences of the resistivity for the above mentioned models of the conduction band of *n*-Ge single-crystals doped by antimony with concentration of $N_d = 5 \cdot 10^{14}$ cm^{-3}.

As the results of the performed experimental investigations show, resistivity for four-valley L_1-model is changed by the law $\rho \sim T^{1.66}$, and for two- and single-valley – by $\rho \sim T^{3/2}$. Such difference in the temperature dependences of the resistivity of *n*-Ge single-crystals at the transition from four- to two- and single-valley L_1-model of the conduction band is obviously connected with the change in contribution at uniaxial pressure of different electron scattering mechanisms. Along with electron scattering by acoustic phonons and impurity ions in *n*-Ge, scattering by optical phonons which is caused by the interaction of electrons with phonons whose frequencies correspond to the temperature of $T_{C1} = 430$ K (intravalley scattering) and intervalley scattering by acoustic phonons with the characteristic temperature of $T_{C2} = 320$ K are also possible [11].

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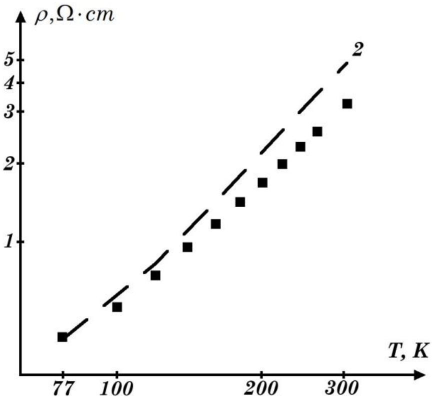

Fig. 1 – Temperature dependence of the resistivity for four-valley L_1-model of the conduction band of n-Ge single-crystal: ■ are the experimental results; 2 is the theoretical calculations using constants of optical $\Xi_{430} = 6.7\cdot 10^8$ eV/cm and intervalley $\Xi_{320} = 1.6\cdot 10^8$ eV/cm strain potentials of the work [11]

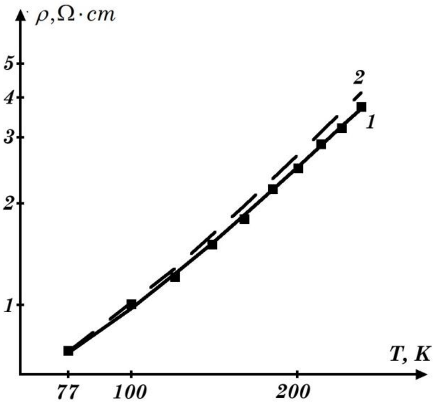

Fig. 2 – Temperature dependence of the resistivity for two-valley L_1-model of the conduction band of n-Ge single-crystal: ■ are the experimental results; 1 is the theoretical calculations using constants of optical $\Xi_{430} = 4\cdot 10^8$ eV/cm and intervalley $\Xi_{320} = 1.4\cdot 10^8$ eV/cm strain potentials; 2 is the theoretical calculations using constants of optical $\Xi_{430} = 6.7\cdot 10^8$ eV/cm and intervalley $\Xi_{320} = 1.6\cdot 10^8$ eV/cm strain potentials of the work [11]

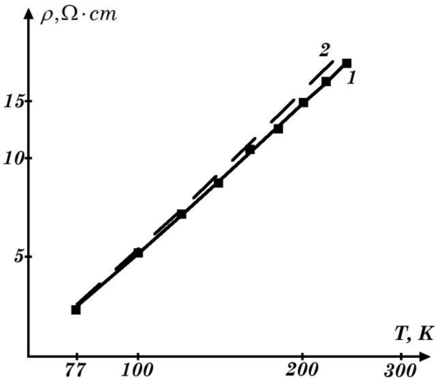

Fig. 3 – Temperature dependence of the resistivity for single-valley L_1-model of the conduction band of n-Ge single-crystal: ■ are the experimental results; 1 is the theoretical calculations using constants of optical $\Xi_{430} = 4\cdot 10^8$ eV/cm and intervalley $\Xi_{320} = 1.4\cdot 10^8$ eV/cm strain potentials; 2 is the theoretical calculations using constants of optical $\Xi_{430} = 6.7\cdot 10^8$ eV/cm and intervalley $\Xi_{320} = 1.6\cdot 10^8$ eV/cm strain potentials of the work [11]

3. THEORETICAL CALCULATIONS OF THE TEMPERATURE DEPENDENCES FOR FOUR-, TWO-, AND SINGLE-VALLEY L_1-MODEL OF THE CONDUCTION BAND OF GERMANIUM SINGLE-CRYSTALS

For quantitative interpretation of the relative contribution of different scattering mechanisms into n-Ge, we have performed theoretical calculations of the given temperature dependences of the resistivity based on the theory of anisotropic scattering [12] (see Fig. 1-Fig. 3, dashed lines 2).

Intervalley electron scattering and electron scattering by optical phonons is described by scalar relaxation time τ_j [11]

$$1/\tau_j = a_j \phi_j , \qquad (1)$$

where

$$a_j = \frac{\Xi_j^2 \left(m_d^j\right)^{3/2}}{\sqrt{2}\pi\rho\hbar^2 \left(kT_{Cj}\right)^{1/2}} \left(\frac{T}{T_{Cj}}\right)^{1/2};$$

$$\phi_j(x) = \frac{1}{e^{T_{Cj}/T}-1}\left[\left(x+\frac{T_{Cj}}{T}\right)^{1/2} + e^{T_{Cj}/T}\theta(x;\frac{T_{Cj}}{T})\left(x-\frac{T_{Cj}}{T}\right)^{1/2}\right];$$

m_d^j is the effective mass of the density of states for the conduction-band electrons; Ξ_j is the constant of intervalley or optical strain potential; ρ is the crystalline density; T_{Cj} is the temperature of the j-th intervalley or optical phonon; $x = \varepsilon/kT$ is the reduced electron energy; $\theta(x;T_{Cj}/T)$ is the step function.

For intervalley scattering

$$m_d^j = \left(m_{\parallel j} m_{\perp j}^2\right)^{1/3}\left(Z_j - 1\right), \qquad (2)$$

where $m_{\parallel j}$ and $m_{\perp j}$ are the longitudinal and transverse components of the effective mass tensor for electrons inside a j-type ellipsoid; Z_j is the number of equivalent ellipsoids of the j-type conduction band.

For intravalley electron scattering by optical phonons

$$m_d^j = \left(m_{\parallel j} m_{\perp j}^2\right)^{1/3} Z_j^{2/3} . \qquad (3)$$

For constant-energy surface, which is an ellipsoid of revolution, charge carrier mobility along an arbitrary direction can be determined from the relation [13]:

$$\mu = \mu_\perp \sin^2\theta + \mu_\parallel \cos^2\theta , \qquad (4)$$

where θ is the angle between the considered direction and ellipsoid principal axis; $\mu_\perp$, $\mu_\parallel$ are the charge carrier mobilities transversely and along the ellipsoid axis.

Then, in accordance with (4), for four-valley L_1-model of the conduction band

$$\mu = \frac{1}{3}\mu_\parallel + \frac{2}{3}\mu_\perp , \qquad (5)$$

for two-valley

$$\mu = \frac{2}{3}\mu_{\|} + \frac{1}{3}\mu_{\perp}, \qquad (6)$$

and for single-valley

$$\mu = \mu_{\|}. \qquad (7)$$

Based on the theory of anisotropic scattering, we write the expressions for $\tau_{\|}$ and $\tau_{\perp}$ in the conditions of mixed scattering by acoustic phonons and impurity ions [12]:

$$\tau_{\|}^{a,i} = \frac{a_{\|}}{\sqrt{k}T^{3/2}} \cdot \frac{x^{3/2}}{x^2 + b_0}, \; \tau_{\perp}^{a,i} = \frac{a_{\perp}}{\sqrt{k}T^{3/2}} \cdot \frac{x^{3/2}}{x^2 + b_1}, \qquad (8)$$

where

$$a_{\|} = \frac{\pi C_{11}\hbar^4}{k\Xi_d^2\sqrt{2m_{\|}m_{\perp}^2}} \cdot \frac{1}{\Phi_{0a}}, \quad a_{\perp} = \frac{\pi C_{11}\hbar^4}{k\Xi_d^2\sqrt{2m_{\|}m_{\perp}^2}} \cdot \frac{1}{\Phi_{1a}}, \qquad (9)$$

$$b_0 = \frac{a_{\|}\cdot\Phi_{0i}}{\sqrt{k}T^{3/2}\tau_{0i}(kT)}, \; b_1 = \frac{a_{\perp}\cdot\Phi_{1i}}{\sqrt{k}T^{3/2}\tau_{0i}(kT)}, \qquad (10)$$

$$\tau_{0i}(kT) = \frac{\sqrt{2}m_{\perp}\varepsilon^2(kT)^{3/2}}{\pi Ne^4\sqrt{m_{\|}}}, \qquad (11)$$

$$\Phi_{1a} = 1 + \frac{1+\beta^2}{\beta^2}\left(2 + \frac{3}{\beta^2} - \frac{3(1+\beta^2)}{\beta^3}\alpha\right)\frac{\Xi_u}{\Xi_d} + \frac{(1+\beta^2)}{\beta^4}\frac{\Xi_u^2}{\Xi_d^2}\left((1+\beta^2)\left(1 + \frac{15}{4\beta^2} - \frac{3}{4\beta^3}(5+3\beta^2)\alpha\right) + \frac{C_{11}}{4C_{44}}\left(-13 - \frac{15}{\beta^2} + \frac{3(1+\beta^2)}{\beta^3}(5+\beta^2)\alpha\right)\right), \qquad (12)$$

$$\Phi_{0a} = 1 + \frac{2(1+\beta^2)}{\beta^2}\left(1 - \frac{3}{\beta^2} + \frac{3}{\beta^3}\alpha\right)\frac{\Xi_u}{\Xi_d} + \frac{(1+\beta^2)}{\beta^4}\frac{\Xi_u^2}{\Xi_d^2}\cdot\left((1+\beta^2)\left(1 - \frac{6}{\beta^2} - \frac{3}{2\beta^2(1+\beta^2)} + \frac{15\alpha}{2\beta^3}\right) + \frac{C_{11}}{C_{44}}\left(2 + \frac{15}{2\beta^2} - \frac{3}{2\beta^3}(5+3\beta^2)\alpha\right)\right), \qquad (13)$$

$$\Phi_{0i} = \frac{3}{2\beta^3}\left(\left(\frac{\beta}{1+\beta^2} - \alpha\right)\ln\gamma^2 - \alpha\ln(1+\beta^2) + 2L(\alpha) + \frac{\beta\gamma^2}{2}\left(\frac{\beta^2-1}{\beta^2+1} + \frac{\alpha(\beta^2+1)}{\beta}\right)\right), \qquad (14)$$

$$\Phi_{1i} = \frac{3}{4\beta^3}\left(\left((1-\beta^2)\alpha - \beta\right)\ln\gamma^2 + 2(\beta^2-1)L(\alpha) - 2\beta^2\alpha - (\beta^2-1)\alpha\ln(1+\beta^2) + \frac{\gamma^2}{2}\left(\beta(1+3\beta^2) + \alpha(3\beta^4 + 2\beta^2 - 1)\right)\right), \qquad (15)$$

where $\alpha = \arctan\beta$, $\beta^2 = \frac{m_{\|} - m_{\perp}}{m_{\perp}}$, $\gamma = \sqrt{\frac{\pi\hbar^2 e^2 N}{2m_{\|}\varepsilon kT}}$, and $L(\alpha) = -\int_0^{\alpha}\ln\cos\phi d\phi$ is the Lobachevsky function, N is the impurity concentration.

Then, in the most general case of electron scattering by acoustic phonons, impurity ions, optical and intervalley phonons, expressions for the components of the relaxation time tensor can be represented as follows:

$$\frac{1}{\tau_{|}} = \frac{1}{\tau_{|}^{a,i}} + \frac{1}{\tau_1} + \frac{1}{\tau_2}; \; \frac{1}{\tau_{\perp}} = \frac{1}{\tau_{\perp}^{a,i}} + \frac{1}{\tau_1} + \frac{1}{\tau_2}, \qquad (16)$$

where $\tau_{|}^{a,i}$, $\tau_{\perp}^{a,i}$, τ_1, τ_2 are the longitudinal and transverse components of the relaxation time tensor for scattering by acoustic phonons and impurity ions; τ_1, τ_2 are the relaxation times for intervalley scattering and scattering by optical phonons.

Components of the mobility tensors can be expressed through the components of the relaxation time and effective mass tensors

$$\mu_{\|} = \frac{e}{m_{\|}}\langle\tau_{\|}\rangle, \; \mu_{\perp} = \frac{e}{m_{\perp}}\langle\tau_{\perp}\rangle. \qquad (17)$$

Then, finally, expressions for the components of the relaxation time tensor will be the following:

$$\langle\tau_{\|}\rangle = \frac{4}{3\sqrt{\pi}}\int_0^{\infty} dx x^{3/2}e^{-x}\tau_{\|}, \quad \langle\tau_{\perp}\rangle = \frac{4}{3\sqrt{\pi}}\int_0^{\infty} dx x^{3/2}e^{-x}\tau_{\perp}. \qquad (18)$$

Resistivity of n-Ge single-crystals is easily expressed through the electron mobility and concentration:

$$\rho = \frac{1}{en\mu}. \qquad (19)$$

Then, based on the correlation (19) and taking into account expressions (1)-(18), one can obtain the temperature dependences of the resistivity for four-, two-, and single-valley L_1-model of the conduction band of n-Ge single-crystals. To this end, one should use all known and surely specified parameters of the L_1-minimum, to which components of the strain potential and effective mass tensors belong ($\Xi_d = -6.4$ eV, $\Xi_u = 16.4$ eV and $m_{\parallel} = 1.58m_0$, $m_{\parallel} = 0.082m_0$) [9]. Also, for the scattering mechanisms we consider, one should additionally have the values of interaction constants between electrons and optical phonons, which correspond to the characteristic temperature $T_{C1} = 430$ K, and intervalley phonons with the temperature of $T_{C2} = 320$ K (constants of the optical and intervalley strain potentials). For the first time the given constants ($\Xi_{430} = 6.7\cdot10^8$ eV/cm and $\Xi_{320} = 1.6\cdot10^8$ eV/cm) were defined based on the Monte Carlo method in the work [11].

The corresponding temperature dependences of the resistivity of n-Ge single-crystals using the given parameters are represented in Fig. 1-Fig. 3 (dashed lines 2). As the performed calculations show, resistivity for the four-valley L_1-model is changed by the law $\rho \sim T^{1.9}$, for two-valley – $\rho \sim T^{1.55}$ and single-valley – $\rho \sim T^{1.63}$ that does not agree with the corresponding experimental dependences. Such discrepancy between the experimental and theoretical dependences is explained by insufficiently precise values of the constants of optical and intervalley strain potential that, as it was mentioned above, requires corrections.

4. DETERMINATION OF THE ELECTRON-PHONON INTERACTION CONSTANTS

In accordance with expressions (1)-(19), components of the relaxation time tensor, and, thus, resistivity, depend on the constants of optical and intervalley strain potential.

Taking into account expressions (1), (5), (8) and (17)-(19) and experimental values of the resistivity for two different temperatures, for example, for four-valley L_1-model of the conduction band of n-Ge single-crystals (Fig. 1, curve 1), we obtain the system of equations for determination of the following constants:

$$\begin{cases} \dfrac{3}{\dfrac{4e^2n}{3\sqrt{\pi}}\left[\dfrac{1}{m_{\parallel}}\int\limits_0^{\infty} dx x^{3/2}e^{-x} f_1(x;T_{Cj};\Xi_j;T_1) + \dfrac{2}{m_{\perp}}\int\limits_0^{\infty} dx x^{3/2}e^{-x} f_2(x;T_{Cj};\Xi_j;T_1)\right]} = \rho(T_1), \\ \dfrac{3}{\dfrac{4e^2n}{3\sqrt{\pi}}\left[\dfrac{1}{m_{\parallel}}\int\limits_0^{\infty} dx x^{3/2}e^{-x} f_1(x;T_{Cj};\Xi_j;T_2) + \dfrac{2}{m_{\perp}}\int\limits_0^{\infty} dx x^{3/2}e^{-x} f_2(x;T_{Cj};\Xi_j;T_2)\right]} = \rho(T_2), \end{cases} \tag{20}$$

where

$$f_1(x;T_{Cj};\Xi_j;T_1) = \frac{\sqrt{k}T_1^{3/2}}{a_{\parallel}}\frac{x^2+b_0}{x^{3/2}} + \sum_{j=1}^{2} a_j(\Xi_j;T_{Cj};T_1)\cdot\phi(T_{Cj};T_1), \tag{21}$$

$$f_2(x;T_{Cj};\Xi_j;T_2) = \frac{\sqrt{k}T_2^{3/2}}{a_{\perp}}\frac{x^2+b_1}{x^{3/2}} + \sum_{j=1}^{2} a_j(\Xi_j;T_{Cj};T_2)\cdot\phi(T_{Cj};T_2). \tag{22}$$

In expressions (21) and (22) the case of $j = 1$ corresponds to optical phonons with the characteristic temperature $T_{C1} = 430$ K and constant of optical strain potential Ξ_{430}, and $j = 2$ – to intervalley phonons with the characteristic temperature $T_{C2} = 320$ K and constant of intervalley strain potential Ξ_{320}.

Solution of the system of equations (20) gives the following values of the electro-phonon interaction constants for optical and intervalley phonons in n-Ge single-crystals: $\Xi_{430} = 4\cdot10^8$ eV/cm, $\Xi_{320} = 1.4\cdot10^8$ eV/cm. Theoretical calculations of the temperature dependences of the resistivity for two- and single-valley L_1-model of the conduction band of n-Ge single-crystals (Fig. 2, Fig. 3, solid lines 1) using the given constants agree well with the obtained experimental results.

5. CONCLUSIONS

Thus, electron scattering by optical and intervalley phonons is important for four-valley L_1-model of the conduction band of n-Ge single-crystals. Electron scattering by acoustic phonons will be the dominant one for the studied impurity concentration for two- and single-valley L_1-model. Use of the electron-phonon interaction constants for optical and intervalley phonons, obtained based on the theory of anisotropic scattering, allows to theoretically describe the features of electron scattering in n-Ge single-crystals and interpret the found experimental results.

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