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ELECTRONIC PROPERTIES OF SEMICONDUCTORS

Electron Scattering in the Δ_1 Model of the Conduction Band of Germanium Single Crystals

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Abstract—Electron scattering in the possible Δ_1 models of the conduction band in germanium crystals formed by hydrostatic or uniaxial pressure is investigated. On the basis of the theory of anisotropic scattering, the temperature dependences of the anisotropy parameter of the relaxation times and electron mobility for these models under conditions of scattering at impurity ions, as well as at acoustic and intervalley phonons are obtained. Analysis of the temperature dependences indicates that, in the temperature range of 77–300 K, intervalley scattering becomes substantial. Only for the Δ_1 model formed by uniaxial pressure along the crystallographic direction [100], the electron scattering at intervalley phonons, which correspond to the *g* transitions, is minor with respect to scattering at acoustic phonons (the intravalley scattering) and impurity ions.

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The development of modern microelectronics and nanoelectronics depends substantially on advances in the physics of semiconductors. Such a semiconductor material as germanium is the raw material for fabricating diodes, triodes, power rectifiers, dosimeter devices, and detectors for dark-matter particles [1, 2]. *n*-type germanium single crystals are now the basic material used as the optical medium for lenses, objectives, and filters, which are used in the spectral range of 3–5 μm and 8–14 μm [3]. Dislocation-free germanium provides a solution to problems, which arise upon the fabrication of nanoscale transistor structures with the use of silicon, which are both stressed and free from large internal mechanical stresses. In particular, the technologies of forming uniaxial deformations in p-type metal–oxide–semiconductor field-effect transistor (nMOSFET) channels in electronic devices makes it possible to increase both the gain and the tunneling current when replacing *n*-Si with *n*-Ge crystals [4–6]. In [7], it was shown that the resistivity of germanium nanowires decreases 30 times at a uniaxial tension strain of 1.8%.

The problem of studying the effect of internal and external deformation fields on the electrical, optical, photoelectric, and magnetic characteristics of such nanostructures and formation on the basis of various elements of functional electronics draws a lot of attention of physicists and technicians working in the field of semiconductor material science. The magnitude of strain fields can be such that, due to reorganization of the band structure of germanium crystals, the involvement of high-energy minima of the germanium conduction band of the type Γ_2, Δ_1, and Γ_{15} in different kinetic and optical effects becomes possible. Also for undeformed *n*-Ge crystals under extreme conditions of the directed action of significant electric, optical, and temperature fields, these high-energy minima can introduce a substantial, and even determining, contribution to the corresponding effects. For example, calculations, which were carried out [8] on the basis of the Monte Carlo method, show that the electron population of the Δ_1 minima of the germanium conduction band can occur even at electric fields with an intensity of $E > 3$–4 kV/cm.

We investigated electron scattering in the Δ_1-model of the conduction band of *n*-Ge:Sb crystals. In [9], it was shown that the energy gap between the L_1 and Δ_1 minima decreases both at hydrostatic pressure and at uniaxial pressure along the [100] and [110] crystallographic directions. In this case, inversion of the L_1–Δ_1 type of an absolute minimum can be implemented at a hydrostatic pressure of about 6 GPa or uniaxial pressures of $X \approx 3$ GPa, when $X \| J \| [100]$, and $X \approx 8$ GPa, when $X \| J \| [110]$. As a result of this, it is possible to obtain the six-ellipsoid Δ_1-model of the conduction band of the *n*-Ge crystals in the case of hydrostatic pressure, and the two-ellipsoid or four-ellipsoid models in the case of uniaxial pressure, respectively. In [10], on the basis of the theory of anisotropic scattering at $T = 77$ K, we obtained the concentration dependences of the electron mobility for these models. However, we considered electron scattering at acoustic phonons and impurity ions in this case. When increasing the temperature, it is necessary to additionally take into account intervalley scattering. For this reason, we considered here the most general case of mixed electron scattering at acoustic phonons (intravalley scat-

tering), impurity ions, and intervalley phonons in these Δ_1 models.

As was shown in [11], intervalley scattering for the Δ_1-minimum is caused by the interaction of electrons with acoustic and optical phonons with frequencies, which correspond to the temperatures $T_{C1} = 320$ K (intervalley scattering of the *f* type), and $T_{C2} = 430$ K, $T_{C3} = 100$ K, (intervalley scattering of the *g* type). Such scattering is described by the scalar relaxation time τ_j:

$$\frac{1}{\tau_j} = \alpha_j \varphi_j, \tag{1}$$

where

$$\alpha_j = \frac{\Theta_j^2 (m_d^j)^{3/2}}{\sqrt{2}\pi\rho\hbar (k T_{Cj})^{1/2}} \left(\frac{T}{T_{Cj}}\right)^{1/2},$$

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

$m_d^j = (m_{\|j} m_{\perp j}^2)^{1/3}(Z^j - 1)$, $m_{\|j}$ and $m_{\perp j}$ are the longitudinal and transverse components of the tensor of effective mass for electrons, which are in the ellipsoid of the *j* type; Z_j is the number of equivalent ellipsoids of the conduction band of the *j* type; Θ_j is the constant of the intervalley-strain potential; ρ is the crystal density; T_{Cj} is the temperature of the *j*th intervalley phonon; $x = \frac{\varepsilon}{kT}$ is the reduced electron energy; and $\theta\left(x; \frac{T_{Cj}}{T}\right)$ is the step function.

The most important parameter, which characterizes the scattering of charge carriers in anisotropic semiconductors, is the parameter of anisotropy of the relaxation times [12]:

$$K_r - \frac{\langle \tau_\| \rangle}{\langle \tau_\perp \rangle}, \tag{2}$$

where $\tau_\|$ and $\tau_\perp$ are the longitudinal and transverse components of the relaxation-time tensor, respectively. Then, under conditions of mixed scattering

$$\frac{1}{\tau_\|} = \frac{1}{\tau_\|^a} + \frac{1}{\tau_\|^i} + \frac{1}{\tau_j}; \quad \frac{1}{\tau_\perp} = \frac{1}{\tau_\perp^a} + \frac{1}{\tau_\perp^i} + \frac{1}{\tau_i}, \tag{3}$$

where $\tau_\|^a$, $\tau_\perp^a$, $\tau_\|^i$, $\tau_\perp^i$ are the longitudinal and transverse components of the relaxation-time tensor for scattering at acoustic phonons (intravalley scattering) and impurity ions, respectively; and τ_j is the relaxation time for intervalley scattering.

On the basis of the theory of anisotropic scattering [13], we have

$$\tau_\|^a = \frac{a_\|}{T\sqrt{kT}\sqrt{x}}, \quad \tau_\perp^a = \frac{a_\perp}{T\sqrt{kT}\sqrt{x}};$$
$$\tau_\|^i = \frac{\tau_{0i}}{\Phi_{0i}}, \quad \tau_\perp^i = \frac{\tau_{0i}}{\Phi_{1i}}. \tag{4}$$

The necessary designations in formulas (4) are given in [10].

Then, finally, the expression for the components of the relaxation-time tensor in the case of a nondegenerate electronic gas has the form:

$$\langle \tau_\| \rangle = \frac{4}{3\sqrt{\pi}} \int_0^\infty dx x^{3/2} e^{-x} \tau_\|,$$
$$\langle \tau_\perp \rangle = \frac{4}{3\sqrt{\pi}} \int_0^\infty dx x^{3/2} e^{-x} \tau_\perp. \tag{5}$$

Taking into account the values of the constants of the deformation acoustic potential and the components of the effective-mass tensor for the Δ_1 minimum [9, 14] ($\Theta_d = -1.7$ eV, $\Theta_u = 12$ eV, $m_\| = 1.65m_0$, $m_\perp = 0.32m_0$), the temperatures of intervalley phonons ($T_{C1} = 320$ K, $T_{C2} = 430$ K and $T_{C3} = 100$ K), and the constants of the deformation intervalley potential Θ_j corresponding to them ($\Theta_{100} = 7.89 \times 10^7$ eV/cm, $\Theta_{320} = 3.27 \times 10^8$ eV/cm, $\Theta_{430} = 1.57 \times 10^8$ eV/cm) [11], the temperature dependences of the parameter of the relaxation-time anisotropy (2) were obtained on the basis of expressions (1)–(5) for the different models of the conduction band of *n*-Ge crystals indicated above. Analysis of these dependences shows that the parameter of relaxation-time anisotropy is almost independent of the temperature for a lightly doped semiconductor in the two-ellipsoid Δ_1 model (Fig. 1, curve *1*). For the four-ellipsoid and six-ellipsoid Δ_1 model, this parameter increases with temperature (Fig. 2, curve *1* and Fig. 3, curve *1*). Such temperature dependences of the parameter of the relaxation-time anisotropy are attributed to the presence of intervalley scattering in these models, the contribution of which increases with temperature. For the two-ellipsoid Δ_1 models, electron scattering at intervalley phonons, which corresponds to the *g* transitions, is minor with respect to scattering at acoustic phonons (intravalley scattering). With increasing doping-impurity concentration, the contribution of the impurity-scattering component also increases together with the considered scattering mechanisms. This affects the increase in the value of the parameter of the relaxation-time anisotropy in these Δ_1 models with increasing impurity concentration.

For comparison of the performed theoretical calculations with experimental results, we obtained the

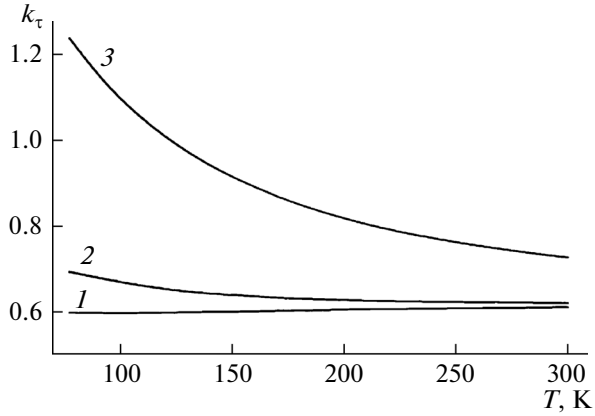

Fig. 1. Temperature dependences of the parameter of the relaxation-time anisotropy for the two-ellipsoid Δ_1 model of the conduction band of germanium crystals formed by uniaxial pressure along the [100] crystallographic direction for the impurity concentration $N_D = (1)\ 10^{13}$, $(2)\ 5 \times 10^{14}$, and $(3)\ 6.6 \times 10^{16}$ cm^{-3}.

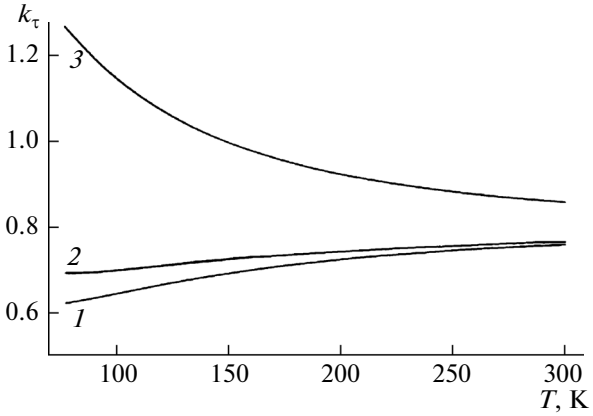

Fig. 2. Temperature dependences of the parameter of the relaxation-time anisotropy for the four- ellipsoid Δ_1 model of the conduction band of germanium crystals in the case of uniaxial pressure along the [110] crystallographic direction for the impurity concentration $N_D = (1)\ 10^{13}$, $(2)\ 5 \times 10^{14}$, and $(3)\ 6.6 \times 10^{16}$ cm^{-3}.

temperature dependences of the resistivity for *n*-Ge single crystals Sb-doped with a concentration of $N_D = 5 \times 10^{14}$ cm^{-3} and uniaxially deformed along the [100] crystallographic direction. Such uniaxial deformation results in synchronous displacement upwards along the energy scale of four L_1 minima and in the lowering of two Δ_1-minima. The uniaxial pressure in the experiments amounted to 2.8 GPa, which enabled us to implement the two-ellipsoid Δ_1 model of the conduction band of *n*-Ge single crystals in a wide temperature range. Taking into account that the electron concentration in the conduction band remains constant and equal to the impurity concentration under these conditions, the corresponding temperature dependences of the electron mobility (Fig. 4, curve *3*) were obtained. At hydrostatic pressure, the four L_1 minima are displaced upwards in terms of energy scale, and six Δ_1 minima move downwards, which enables us to obtain the six-ellipsoid Δ_1 model of the conduction band of *n*-Ge single crystals at a pressure of about 6 GPa. Taking into account this fact, the authors of [15] obtained the experimental results of the temperature dependences of electron mobility for this Δ_1 model (Fig. 4, curve *2*a) on the basis of the measurements of the piezo–Hall effect at hydrostatic pressure. In the case of uniaxial pressure along the [110] crystallographic direction, the two L_1 minima and four Δ_1 minima are displaced downwards in terms of energy scale. Since the value of the pressure coefficient for four Δ_1 minima is larger than that for two L_1 minima at a pressure of about 8 GPa, as was shown in [9], it is possible to implement inversion of the L_1–Δ_1 type of the absolute minimum and to obtain the four-ellipsoid Δ_1 model of the conduction band in the *n*-Ge single crystals. To carry out measurements of the temperature dependences of the resistivity at such a large uniaxial-pressure value is almost an insoluble experimental problem because its value is close to the critical pressure value, when there is a loss in the germanium-sample stability. Therefore, we restrict ourselves only to theoretical calculations (Fig. 4, curves *1* and *1*′).

As is known, the isoenergetic surfaces for both L_1 and the Δ_1 minima are ellipsoids of revolution. Then, the mobility of charge carriers in an arbitrary direction can be determined from the relation [16]

$$\mu = \mu_\perp \sin^2\theta + \mu_\parallel \cos^2\theta, \qquad (6)$$

where θ is the angle between the direction under consideration and the principal axis of the ellipsoid; $\mu_\parallel$ and

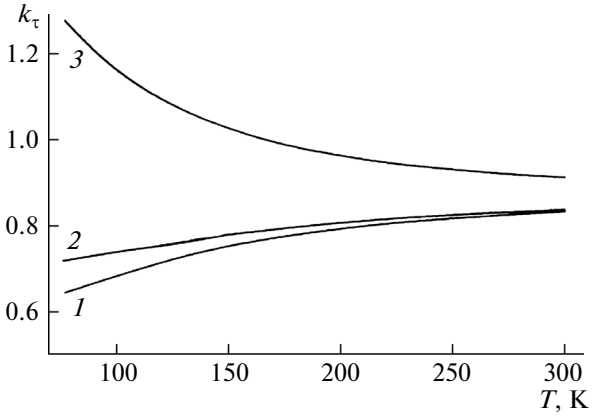

Fig. 3. Temperature dependences of the parameter of the relaxation-time anisotropy for the six-ellipsoid Δ_1 model of the conduction band of germanium crystals in the case of hydrostatic pressure for the impurity concentration $N_D = (1)\ 10^{13}$, $(2)\ 5 \times 10^{14}$, and $(3)\ 6.6 \times 10^{16}$ cm^{-3}.

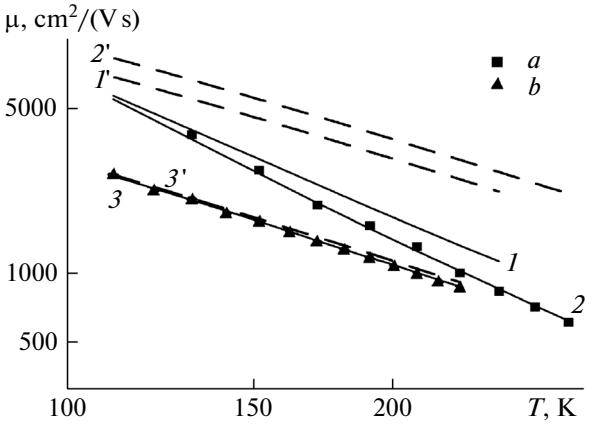

Fig. 4. Temperature dependences of the electron mobility for the Δ_1 minimum of the conduction band of *n*-Ge crystals: (*1*) in the case of uniaxial pressure along the [110] crystallographic direction, (*2*) in the case of hydrostatic pressure, (*3*) in the case of uniaxial pressure along the [100] crystallographic direction; (*a*) experimental results for the electron concentration $n = N_D - N_A = 4.72 \times 10^{13}$ cm^{-3} [15]; (*b*) our experimental results for the electron concentration $n = N_D = 5 \times 10^{14}$ cm^{-3}. Solid lines are the results of theoretical calculations with intervalley scattering taken into account, and the dashed lines are theoretical results obtained with this scattering disregarded.

$\mu_\perp$ are the charge-carrier mobilities across and along the ellipsoid axis, respectively. According to expression (1), for the Δ_1 minimum,

$$\mu^{\Delta_1} = \mu_\parallel^{\Delta_1} \quad (7)$$

in the case of uniaxial pressure along the [100] crystallographic direction and

$$\mu^{\Delta_1} = \frac{1}{2}\mu_1^{\Delta_\parallel} + \frac{1}{2}\mu_\perp^{\Delta_1}, \quad (8)$$

when the uniaxial pressure is directed along the [110] crystallographic direction.

In the case of hydrostatic pressure,

$$\mu^{\Delta_1} = \frac{1}{3}\mu_\parallel^{\Delta_1} + \frac{2}{3}\mu_\perp^{\Delta_1}. \quad (9)$$

On the other hand, the components of the mobility tensors can be expressed in terms of components of the relaxation-time tensor and the effective-mass tensor:

$$\mu_\parallel^{\Delta_1} = \frac{e}{m_\parallel^{\Delta_1}}\langle\tau_\parallel^{\Delta_1}\rangle, \quad \mu_\perp^{\Delta_1} = \frac{e}{m_\perp^{\Delta_1}}\langle\tau_1^{\Delta_1}\rangle. \quad (10)$$

Taking into account the above values of constants of the deformation potential and components of the effective-mass tensor, we used expressions (7)–(10) to obtain the temperature dependences of the electron mobility for the Δ_1 minimum with consideration and disregarding intervalley scattering (Fig. 4, solid and dashed curves). The obtained results of theoretical calculations and experimental investigations show that the electron mobility varies by the law $\mu \sim T^{-2.27}$ for the six-ellipsoid Δ_1 model, $\mu \sim T^{-1.98}$ for the four-ellipsoid model, and $\mu \sim T^{-1.53}$ for the two-ellipsoid model. The temperature dependence of the electron mobility for the two-ellipsoid Δ_1 model of the conduction band of the *n*-Ge crystals corresponds to the typical law of electron scattering at acoustic phonons $\mu \sim T^{-1.5}$. The increase in the exponent in the temperature dependence of the electron mobility $\log\mu = f(\log T)$ for the four-ellipsoid and six-ellipsoid Δ_1 models is attributed to the presence of an additional mechanism of intervalley scattering in these cases.

The performed theoretical and experimental investigations enable us to formulate the following conclusions.

(i) Electron scattering in the Δ_1 models of the conduction band of germanium crystals is anisotropic.

(ii) The results of theoretical calculations of the electron mobility with and without taking into account intervalley scattering show that it is intervalley scattering that is substantial for the six-ellipsoid and four-ellipsoid Δ_1 models of the *n*-Ge conduction band in the temperature range of 77–300 K. Only for the Δ_1 model, formed by uniaxial pressure along the [100] crystallographic direction, is electron scattering at the intervalley phonons corresponding to the *g* transitions minor with respect to scattering at acoustic phonons (intravalley scattering) and impurity ions.

(iii) Analysis of the temperature dependences of the electron mobility and the parameter of relaxation-time anisotropy for the four-ellipsoid and six-ellipsoid Δ_1 model shows that the efficiency of the intervalley scattering is also affected by the Δ_1-band structure itself, i.e., the number of equivalent ellipsoids, which form it.

(iv) The obtained results can be used in designing and modeling the necessary elements of microelectronics and nanoelectronics on the basis of *n*-Ge, which operate under conditions of significant deformation fields.

REFERENCES

1. A. A. Selesniov, A. Y. Aleinikov, P. V. Ermakov, N. S. Ganchuk, S. N. Ganchuk, and R. E. Jones, Phys. Solid State **54**, 436 (2012).
2. S. W. Leman, S. A. Hertel, P. Kim, B. Cabrera, E. do Couto e Silva, E. Figueroa-Feliciano, K. A. McCarthy, R. Resch, B. Sadoulet, and K. M. Sundqvist, J. Low Temp. Phys. **166**, 1106 (2012).
3. A. P. Oksanich and V. V. Malevannyi, Vestn. Kremenchug. Nats. Univ. Ostrogradskogo **78** (1), 18 (2013).

4. M. Kobayashi, A. Kinoshita, K. Saraswat, H.-S. P. Wong, and Y. Nishi, Electron Dev. **57**, 1037 (2010).
5. M. Kobayashi, T. Irisawa, B. M. Kope, Yun Sun, K. Saraswat, H.-S. P. Wong, P. Pianetta, and Y. Nishi, in *Proceedings of the Symposium on VLSI Technology* (2009), p. 76.
6. Choi Youn Sung, Lim Ji-Song, Numata Toshinori, Nishida Toshikazu, and E. S. Thompson, J. Appl. Phys. **102**, 104507 (2007).
7. J. Greil, A. Lugstein, C. Zeiner, G. Strasser, and E. Bertagnolli, Nano Lett. **12**, 6230 (2012).
8. C. Jacoboni, F. Nava, C. Canali, and G. Ottaviani, Phys. Rev. B **24**, 1014 (1981).
9. S. V. Luniov, P. F. Nazarchuk, and O. V. Burban, in *Proceedings of the 6th International Scientific Conference RNAOPM* (Lutsk, Ukraine, 2012), p. 42.
10. S. V. Luniov, P. F. Nazarchuk, and O. V. Burban, Semiconductors **48**, 438 (2014).
11. W. Fawcett and E. G. S. Paige, J. Phys. C: Solid State Phys. **4**, 1801 (1971).
12. C. Herring and E. Vogt, Phys. Rev. **101**, 944 (1956).
13. P. I. Baranskii, I. S. Buda, I. V. Dakhovskii, and V. V. Kolomoets, *Electrical and Galvanomagnetic Phenomena in Anisotropic Semiconductors* (Naukova Dumka, Kiev, 1977), p. 269 [in Russian].
14. S. V. Luniov, P. F. Nazarchuk, and O. V. Burban, J. Phys. Study **3**, 3702 (2013).
15. C. N. Ahmad and A. R. Adams, Phys. Rev. B **34**, 2319 (1986).
16. G. L. Bir and G. E. Pikus, *Symmetry and Stain-Induced Effects in Semiconductors* (Wiley, New York, 1975), p. 584.

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