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Influence of mutual drag of light and heavy holes on conductivity of *p*-silicon and *p*-germanium

I.I. Boiko
V. Lashkaryov Institute of Semiconductor Physics, NAS of Ukraine
45, prospect Nauky, 03028 Kyiv, Ukraine
E-mail: igorboiko@yandex.ru
Phone: +38 (044)236-5422

Abstract. Conductivity of *p*-Si and *p*-Ge is considered for the two-band model with due regard for mutual drag of light and heavy holes. It is shown that for small and moderate temperatures this drag significantly diminishes the drift velocity of light holes and, as a result, the whole conductivity of crystal. The drag effect considered here appears also in the form of non-monotonous dependences of conductivity on temperature and carrier concentration.

Keywords: silicon, germanium, balance equation, conductivity, drag.

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1. Introduction

In previous work, we investigated direct influence of inter-electron interaction on conductivity of *n*-silicon [1]. In contrast to crystals with one simple band, where the electron-electron scattering does not change the total momentum of carriers, in multivalley crystals the conductivity can be essentially influenced by mutual drag of carriers that belong to different partial bands or valleys (see Refs. [1, 2]). The analogous effect has to appear in semiconductors where band carriers occupy several subbands, and transitions between these subbands are sufficiently rare. If mobilities of carriers from separate subbands are appreciable, then values of separate drift flows are determined not only by external scattering system (phonons, impurities) but by mutual drag, too. In this case, the more quick flow is inhibited by the more slow flow, and the latter is accelerated by the former one. This drag changes the total conductivity of crystal.

Convenient objects to investigate this mutual drag are *p*-silicon and *p*-germanium. We consider here the two-band model for these crystals and for simplicity of calculations accept spherical band approximation. So, the dispersion law has the following simple form:

$$\varepsilon_{\vec{k}}^{(a)} = \hbar^2 k^2 / 2m_a \quad (a = 1 \text{ or } 2). \tag{1}$$

Here, m_a are effective masses (m_1 is the mass of light holes, and m_2 is the mass of heavy holes).

Previous calculations show that approximation of spherical bands introduces into the calculated conductivity some inaccuracy about several percents only. The considered mutual drag can change conductivity much more.

In the case $m_1 << m_2$, the concentration of light holes p_1 differs substantially from the concentration of heavy holes p_2 (see Ref. [3]). We have $\frac{p_2}{p_1} = \left(\frac{m_2}{m_1}\right)^{3/2} = \left(\frac{0.33m_0}{0.04m_0}\right)^{3/2} = 23.7$ for *p*-germanium and $\frac{p_2}{p_1} = \left(\frac{m_2}{m_1}\right)^{3/2} = \left(\frac{0.56m_0}{0.16m_0}\right)^{3/2} = 6.55$ for *p*-silicon. One can see that the concentration of light holes is small and they cannot drag heavy holes noticeably. Therefore, heavy holes are not sensitive to the drag by light holes. We have a quite opposite situation for light holes. In spite of small number, their contribution to the total conductivity is quite comparable with contribution of heavy holes. Therefore, drag of light holes by heavy holes can influence essentially on the total conductivity.

2. Balance equations

Many years ago (see Ref. [3]), some special attempt was taken to consider influence of intervalley scattering on cyclotron resonance in silicon. Performing their calculations, the authors of this article followed directions of Ref. [4] where additional scattering term for kinetic equation (in the form of tau-approximation) was proposed. It was not good idea, because collision integral for $e-e$-scattering principally cannot represent in the form containing some relaxation time (see Ref. [5]).

We use here a quite another approach that allows to involve into consideration interaction of band carriers with good reasons (see, for example, Refs. [6, 7]).

We begin consideration of the conductivity from the set of two balance equations obtained as a first momentum of quantum kinetic equations (see Refs [2, 7]):

$$e\,\vec{E}+\vec{F}^{(a)}+\sum_{b=1}^{2}\vec{F}^{(a,b)}=0 \quad (a=1,2). \tag{2}$$

Here, $\vec{E}$ is the applied electric field; the resistant force related to an external scattering system is

$$\vec{F}^{(a)}=-\frac{e^2}{(2\pi)^6 p_a}\int d^3\vec{k}\int \vec{q}d^3\vec{q}\int d\omega\,\delta(\hbar\omega-\varepsilon_{\vec{k}}^{(a)}+\varepsilon_{\vec{k}-\vec{q}}^{(a)})\times$$
$$\times\{f_{\vec{k}}^{(a)}-f_{\vec{k}-\vec{q}}^{(a)}+[f_{\vec{k}}^{(a)}(1-f_{\vec{k}-\vec{q}}^{(a)})+$$
$$+f_{\vec{k}-\vec{q}}^{(a)}(1-f_{\vec{k}}^{(a)})]\tanh(\hbar\omega/2k_BT)\}[\langle\varphi_{(I)}^2\rangle_{\omega,\vec{q}}+\langle\varphi_{(ph)}^2\rangle_{\omega,\vec{q}}]. \tag{3}$$

We consider here interaction of holes with acoustic phonons and charged impurities disposed uniformly in space. In Eq. (3), the value $f_{\vec{k}}^{(a)}$ is non-equilibrium distribution function for a-holes; the values $\langle\varphi_{(I)}^2\rangle_{\omega,\vec{q}}$ and $\langle\varphi_{(ph)}^2\rangle_{\omega,\vec{q}}$ are Fourier components of correlator of impurity and phonon scattering potentials. In our calculations, we use such forms (see Refs. [2, 7]):

$$\langle\varphi_{(I)}^2\rangle_{\vec{q},\omega}=\frac{32\pi^3e^2n_I}{|\varepsilon(\omega=0,\vec{q})|^2q^4}\delta(\omega); \tag{4}$$

$$\langle\delta\varphi_{(ph)}^2\rangle_{\vec{q},\omega}=\Xi_A^2\frac{2\pi k_BT}{e^2\rho s^2}\delta(\omega). \tag{5}$$

Here n_I is the concentration of charged impurities, Ξ_A is the deformation potential constant. The form (5) corresponds to the approximation of quasi-elastic collisions.

The screening dielectric function for quasi-elastic collisions we take in the form

$$\varepsilon(\omega,\vec{q})=\varepsilon_L(1+q_0^2/q^2), \tag{6}$$

where ε_L is the dielectric constant of crystal lattice. For nondegenerate carriers

$$q_0^2=\frac{4\pi e^2(p_1+p_2)}{\varepsilon_Lk_BT}. \tag{7}$$

The Coulomb interaction between all holes is presented by the forces (a, b = 1, 2)

$$\vec{F}^{(a,b)}=\frac{e^4\hbar}{4\pi^6p_a}\int\vec{k}\,d^3\vec{k}\int d^3\vec{k}'\times$$
$$\times\int d^3\vec{q}\,\frac{1}{q^4}\frac{\delta(\varepsilon_{\vec{k}}^{(a)}-\varepsilon_{\vec{k}-\vec{q}}^{(a)}-\varepsilon_{\vec{k}'}^{(b)}+\varepsilon_{\vec{k}'-\vec{q}'}^{(b)})}{|\varepsilon(\omega=0,\vec{q})|^2}\mathrm{Y}_{ab}(\vec{k},\vec{k}',\vec{q});$$
$$Y_{ab}(\vec{k},\vec{k}',\vec{q})=f_{\vec{k}-\vec{q}}^{(a)}(1-f_{\vec{k}}^{(a)})f_{\vec{k}'}^{(b)}(1-f_{\vec{k}'-\vec{q}}^{(b)})-$$
$$-f_{\vec{k}}^{(a)}(1-f_{\vec{k}-\vec{q}}^{(a)})f_{\vec{k}'-\vec{q}}^{(b)}(1-f_{\vec{k}'}^{(b)}). \tag{8}$$

To calculate the drift velocities $\vec{u}^{(a)}$ of electrons from a-group we accept the model of non-equilibrium distribution functions as Fermi functions with argument containing shift of velocity $\vec{v}^{(a)}(\vec{k})=\hbar^{-1}(\partial\varepsilon_{\vec{k}}^{(a)}/\partial\vec{k})$ on the corresponding velocity $\vec{u}^{(a)}$:

$$f_{\vec{k}}^{(a)}=f^{0(a)}(\vec{v}^{(a)}(\vec{k})-\vec{u}^{(a)}) \qquad (a=1,2). \tag{9}$$

Here, $f^{0(a)}(\vec{v}^{(a)}(\vec{k}))=f_0{}^{(a)}(\varepsilon)$ is the equilibrium distribution function for a-carriers. The drift velocities $\vec{u}^{(a)}$ are proportional to partial densities of currents $\vec{j}^{(a)}$:

$$\vec{u}^{(a)}=\frac{1}{ep_a}\vec{j}^{(a)}. \tag{10}$$

The density of total current is

$$\vec{j}=\sum_{a=1}^{2}\vec{j}^{(a)}. \tag{11}$$

Using the forms (9) and carrying out linearization of forces in Eqs. (2) over drift velocities, for spherical symmetry we obtain the following set of balance equations:

$$\vec{F}^{(a)}=-e\beta^{(a)}\vec{u}^{(a)};\ \vec{F}^{(a,b)}=-e\,\xi^{(a,b)}\left(\vec{u}^{(a)}-\vec{u}^{(b)}\right). \tag{12}$$

Here, the coefficients $\beta^{(a)}$ and $\xi^{(a,b)}$ are (see Refs [2, 7]):

$$\beta^{(a)}=\lambda^{(a)}+\chi^{(a)}; \tag{13}$$

$$\lambda^{(a)}=\frac{\hbar}{6(2\pi)^5e\;p^{(a)}k_BT}\int d\omega\times$$
$$\times\int\frac{q^4d^3\vec{q}}{\sinh(\hbar\omega/k_BT)}\mathrm{Im}\Delta\varepsilon_{(a)}^0(\omega,\vec{q})\langle\varphi_{(I)}^2\rangle_{\omega,\vec{q}}=$$
$$=\frac{en_I}{6\pi^2\;p^{(a)}\varepsilon_L^2}\int\left[\frac{1}{\omega}\mathrm{Im}\Delta\varepsilon_{(a)}^0(\omega,\vec{q})\right]_{\omega=0}\frac{q^4}{[q^2+q_0^2(\vec{q})]^2}d^3\vec{q}; \tag{14}$$

$$\chi^{(a)}=\frac{\hbar}{6(2\pi)^5e\;p^{(a)}k_BT}\int d\omega\times$$
$$\times\int\frac{q^4d^3\vec{q}}{\sinh(\hbar\omega/k_BT)}\mathrm{Im}\Delta\varepsilon_{(a)}^0(\omega,\vec{q})\langle\varphi_{(ph)}^2\rangle_{\omega,\vec{q}}=$$
$$=\frac{\Xi_A^2k_BT}{96\pi^4p^{(a)}e^3\rho s^2}\int\left[\frac{1}{\omega}\mathrm{Im}\Delta\varepsilon_{(a)}^0(\omega,\vec{q})\right]_{\omega=0}q^4d^3\vec{q}; \tag{15}$$

$$\xi^{(a,b)} = \frac{\hbar^2(1-\delta_{ab})}{6(2\pi)^4 e\, \varepsilon_L^2 p^{(a)} k_B T} \int \frac{d\omega}{\sinh^2(\hbar\omega/2k_B T)} \times$$
$$\times \int \frac{q^6 d^3\vec{q}}{[q^2+q_0^2(q)]^2} \mathrm{Im}\Delta\varepsilon^0_{(a)}(\omega,\vec{q})\,\mathrm{Im}\Delta\varepsilon^0_{(b)}(\omega,\vec{q})\,. \tag{16}$$

In Eqs. (14)-(16), the imaginary part of dielectric function is presented by the expression

$$\mathrm{Im}\Delta\varepsilon^{\,0}_{(a)}\,(\omega\,,\vec{q}) = -\frac{e^2}{\pi q^2}\int d^3\vec{k}[f_0(\varepsilon^{(a)}_{\vec{k}}) - f_0(\varepsilon^{(a)}_{\vec{k}-\vec{q}})]\times$$
$$\times\delta(\varepsilon^{(a)}_{\vec{k}-\vec{q}} - \varepsilon^{(a)}_{\vec{k}} + \hbar\omega)\,. \tag{17}$$

For quasi-elastic collisions, we have the form (see Ref. [2])

$$\mathrm{Im}\Delta\varepsilon^{(0)}_{(a)}(\omega\to 0,\vec{q}) = \omega\Lambda^{(a)}(\vec{q})\,,$$

where

$$\Lambda^{(a)}(\vec{q}) = \frac{2e^2\, m_a^2}{q^3\hbar^3}\left[1+\exp\left\{\frac{\hbar^2 q^2}{8k_B T\, m_a} - \eta\right\}\right]^{-1}. \tag{18}$$

Here, η is the dimensionless Fermi-energy: $\eta = \varepsilon_F / k_B T$.

As a result, we have for non-degenerate holes:

$$\lambda^{(a)} = \frac{4\sqrt{2\pi m_a}\, e^3\, n_I}{3(k_B T)^{3/2}\varepsilon_L^2}\int_0^\infty \frac{q^3 dq}{[q^2+q_0^2(\vec{q})]^2}\exp\left(-\frac{\hbar^2 q^2}{8m_a k_B T}\right), \tag{19}$$

$$\chi^{(a)} = \frac{8\sqrt{2}\,\Xi_A^2 (k_B T)^{3/2} m_a^{5/2}}{3\pi^{3/2}\hbar^4 e\rho\, s^2}\,, \tag{20}$$

$$\xi^{(a,b)} = \frac{8\gamma e^3\, m_b^2 p_a}{3k_B T\hbar m_a}\times$$
$$\times\int_0^\infty \frac{q^2 dq}{[q^2+q_0^2(q)]^2}\exp\left[-\frac{\hbar^2 q^2}{8k_B T}\left(\frac{1}{m_1}+\frac{1}{m_2}\right)\right], \tag{21}$$

where

$$\gamma = \int_{-\infty}^{\infty}\frac{w^2 dw}{\sinh^2 w}\approx 3.29. \tag{22}$$

Note that

$$p_a\xi^{(a,b)} = p_b\xi^{(b,a)}\,. \tag{23}$$

Therefore, $\xi^{(2,1)} = (p_1/p_2)\xi^{(1,2)} \equiv w\xi^{(1,2)}$.

Farther, we use the designation $\xi^{(1,2)} = \xi$. For germanium, $w = 0.042$; for silicon, $w = 0.153$ (see Ref. [8]). We also assume $n_I = p = p_1 + p_2$.

As a result, we have the following system for drift velocities of light and heavy holes:

$$\vec{E} = \beta^{(1)}\vec{u}_1 + \xi(\vec{u}_1 - \vec{u}_2);\;\; \vec{E} = \beta^{(2)}\vec{u}_2 + w\xi(\vec{u}_2 - \vec{u}_1)\,. \tag{24}$$

The case $\xi = 0$ corresponds to neglecting the mutual drag of light and heavy holes.

3. Mobility of holes

Solving the system (24), one obtains the following expressions for drift velocities of light and heavy holes:

$$\vec{u}_1(\xi) = \frac{\beta^{(2)} + (w+1)\xi}{\beta^{(1)}\beta^{(2)} + \xi(\beta^{(2)} + w\beta^{(1)})}\vec{E} \equiv \mu_1(\xi)\vec{E}\,;$$
$$\vec{u}_2(\xi) = \frac{\beta^{(1)} + (w+1)\xi}{\beta^{(1)}\beta^{(2)} + \xi(\beta^{(2)} + w\beta^{(1)})}\vec{E} \equiv \mu_2(\xi)\vec{E}. \tag{25}$$

Thereof, one finds the dependences of drift velocities on the drag coefficient ξ. For relative values

$$\frac{u_1(\xi)}{u_1(0)} = \frac{\beta^{(1)}[\beta^{(2)} + (w+1)\xi]}{\beta^{(1)}\beta^{(2)} + \xi(\beta^{(2)} + w\beta^{(1)})};$$
$$\frac{u_2(\xi)}{u_2(0)} = \frac{\beta^{(2)}[\beta^{(1)} + (w+1)\xi]}{\beta^{(1)}\beta^{(2)} + \xi(\beta^{(2)} + w\beta^{(1)})}. \tag{26}$$

Let us introduce the total conductivity $\sigma(\xi)$ and the hole mobility $\mu(\xi)$ by using the following relations:

$$\sigma(\xi) = \frac{e}{E}[p_1 u_1(\xi) + p_2 u_2(\xi)]\;;$$
$$\mu(\xi) = \frac{\sigma(\xi)}{p_1 + p_2} = \frac{\sigma(\xi)}{p}\,. \tag{27}$$

4. Results of numerical calculations

In this work, our numerical calculations have been performed for non-degenerate holes. Fig. 1 shows areas substantially different in relation to degeneracy. Presented there separating lines correspond to the case $\varepsilon_F = 0$.

To perform numerical calculations, we used the following values:

$\varepsilon_L = 12$, $\rho s^2 = 1.66\cdot 10^{11}\,\mathrm{Pa}$, $\Xi_A = -4.2\,\mathrm{eV}$ for *p*-silicon and

$\varepsilon_L = 16$, $\rho s^2 = 1.26\cdot 10^{11}\,\mathrm{Pa}$, $\Xi_A = 1.9\,\mathrm{eV}$ for *p*-germanium.

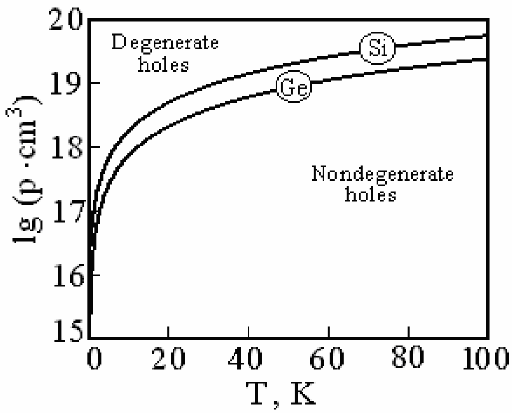

Fig. 1. Areas of degenerate and nondegenerate holes.

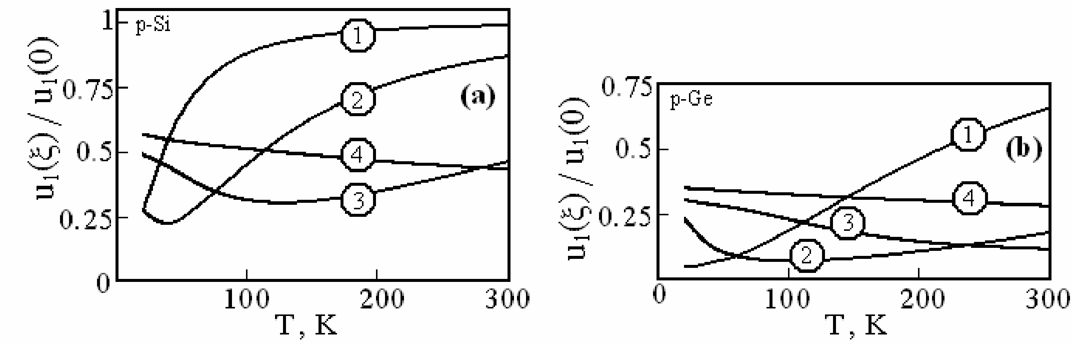

Fig. 2. Dependence of the relative drift velocity for light holes on temperature for $p-\mathrm{Si}$ (a) and $p-\mathrm{Ge}$ (b). $p = 10^{12}\,\mathrm{cm}^{-3}$ (*1*); $10^{14}\,\mathrm{cm}^{-3}$ (*2*); $10^{16}\,\mathrm{cm}^{-3}$ (*3*); $10^{18}\,\mathrm{cm}^{-3}$ (*4*).

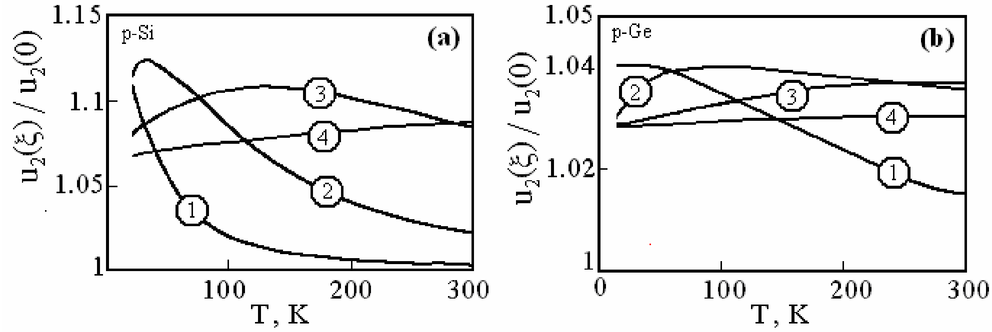

Fig. 3. Dependence of the relative drift velocity for heavy holes on temperature for $p-\mathrm{Si}$ (a) and $p-\mathrm{Ge}$ (b). $p = 10^{12}\,\mathrm{cm}^{-3}$ (*1*); $10^{14}\,\mathrm{cm}^{-3}$ (*2*); $10^{16}\,\mathrm{cm}^{-3}$ (*3*); $10^{18}\,\mathrm{cm}^{-3}$ (*4*).

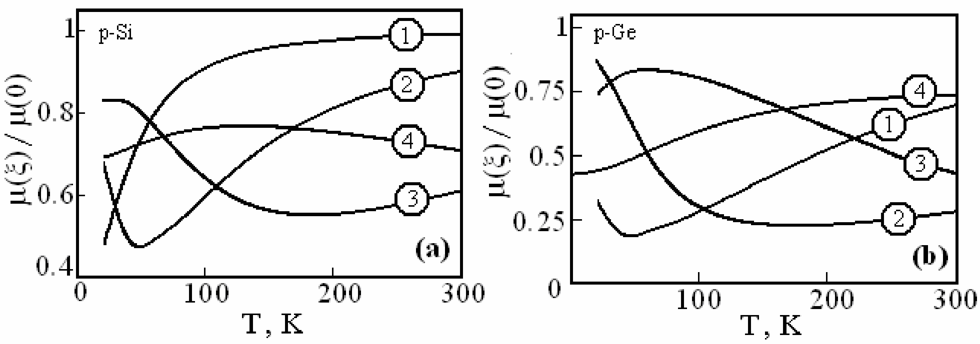

Fig. 4. Dependence of the relative mobility on temperature for $p-\mathrm{Si}$ (a) and $p-\mathrm{Ge}$ (b). $p = 10^{12}\,\mathrm{cm}^{-3}$ (*1*); $10^{14}\,\mathrm{cm}^{-3}$ (*2*); $10^{16}\,\mathrm{cm}^{-3}$ (*3*); $10^{18}\,\mathrm{cm}^{-3}$ (*4*).

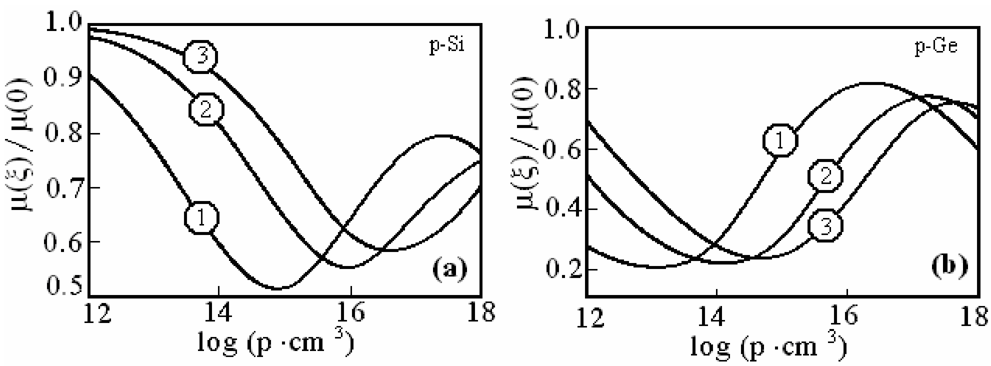

Fig. 5. Dependence of the relative mobility on the hole concentration for $p-\mathrm{Si}$ (a) and $p-\mathrm{Ge}$ (b). $T =$ 100 K (*1*), 200 K (*2*), 300 K (*3*).

Figs. 2a, b show relation of light hole drift velocities calculated for dragged (there we have $u_1(\xi)$) and for undragged carriers (there we have $u_1(0)$). It is evident that mutual drag significantly diminishes (by several times) the drift velocity of light holes.

Figs. 3a, b allow to visually compare the heavy hole drift velocities calculated for dragged and undragged carriers. One can see that drag by light holes increases the drift velocity of heavy holes only by few percents.

Figs. 4a, b and 5a, b demonstrate level of influence of mutual drag of light and heavy holes on the total conductivity of *p*-silicon and *p*-germanium. The main result of carried calculations is the absolute decrease of total conductivity due to mutual drag. It should point out the complicated dependences of the ratio $\sigma(\xi)/\sigma(0)$ on temperature and on total concentration of holes.

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