Influence of electron - phonon interaction on piezoresistance of single crystals n-Ge

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ABSTRACT

Piezoresistance of uniaxially deformed along the crystallographic direction [100] single crystals *n-Ge* for different fixed temperatures has been investigated. Presence of the significant piezoresistance for given conditions of the experiment is explained by increase in the effective mass and decrease in the relaxation time for electrons at the expense of the inversion of (L_1-Δ_1) type of an absolute minimum in *n-Ge*. Temperature dependencies of resistivity for undeformed (L_1 model of conduction band) and deformed under uniaxial pressure *P=3 GPa* (Δ_1 model of conduction band) single crystals *n-Ge* are obtained. Resistivity for undeformed single crystals *n-Ge* is changed according to the law $\rho \sim T^{1.66}$. Resistivity for uniaxially deformed single crystals *n-Ge* is changed as $\rho \sim T^{1.53}$. The given dependencies show that for L_1 model of the conduction band in contrast to Δ_1 model one must equally with intravalley scattering of electrons on acoustic phonons take into account scattering of electrons on optical and intervalley phonons. Therefore reduction of the magnitude piezoresistance n-Ge with the increasing temperature is associated with "turning-off" at the expense of the inversion of (L_1-Δ_1) type of absolute minimum under uniaxial pressure *P>2.7 GPa* mechanism for scattering of electrons on intervalley and optical phonons. Comparison of results of theoretical calculations with relevant experimental data shows that peculiarities of piezoresistance *n-Ge* under uniaxial pressures *1.6<P<2.7 GPa* for (L_1-Δ_1) model of conduction band *n-Ge* can be described only taking into account nonequivalent intervalley scattering of electrons between the minima L_1 and Δ_1.

Keywords: Piezoresistance of single crystals n-Ge; Uniaxial deformation; Intervalley scattering.

INTRODUCTION

Monocrystalline germanium is widely used as a raw material for the manufacture of different kinds of semiconductor devices such as diodes, triodes, power rectifiers, dosimetric devices, optical elements of infrared technique [1]. Hot electrons in *n-Ge* is a source of terahertz radiation, which is widely used in engineering, medicine [2]. Optical and electrical properties of multivalley semiconductors depend significantly on lattice strain. Sharp growth of the intensity of exciton absorption in crystals of germanium under hydrostatic pressure more than *0.6 GPa* has been revealed in work [3]. The authors of the work [4] showed that the life time of excitons in germanium depends on the hydrostatic pressure and intervalley scattering of electrons between the minima of conduction band of different symmetry. Strained germanium is also a promising material for Nan electronics. Elastic fields of deformation on the boundary of heterojunction in *Si/Ge* heterostructures arise due to the discrepancy of lattice constant of germanium and silicon [5]. The use of nanostructures with the self-induced *Ge/Si* Nan islands starts the new prospects for the development of opto- and Nan electronics [6]. The spatial arrangement of these Nan islands depends on the distribution of deformation fields in these nanostructures [7]. That's why the study of different kinetic and optical effects in the deformed single crystals *n-Ge* is actual both in the theoretical and applied sense.

Experimental and theoretical calculations for a wide temperature range show that the effect of piezoresistance *n-Ge*, which is associated with deforming redistribution of electrons between the minima of *L₁* type (effect Smith – Herrìng piezoresistance) will be no longer missed under uniaxial pressures *P > 1.5 GPa* [8]. Giant piezoresistance in *n-Ge* under uniaxial pressure *P>2.1 GPa* along the crystallographic direction in [100] was first experimentally achieved in [9]. In this case was obtained a deformationally-induced phase transition metal-nonconductor which is associated with deforming redistribution of electrons between the minima of *L₁* and *Δ₁* type with different effective mass and emergence due to the uniaxial pressure of energy gap between the admixture area and conduction band. Resistivity and Hall coefficient *n-Ge* with double-charging deep level of gold depending on the hydrostatic pressure at room temperature has been investigated in work [10]. Obtained experimental results are explained by the authors with the presence of intervalley scattering between the minima *L₁* and *Δ₁*.

EXPERIMENTAL RESULTS

We investigated piezoresistance of single crystals *n-Ge* which had been alloyed by the impurity Sb with concentration $N_D=5\cdot10^{14}$ cm^3 under uniaxial pressure along the crystallographic direction [100] for different fixed temperatures (fig. 1).
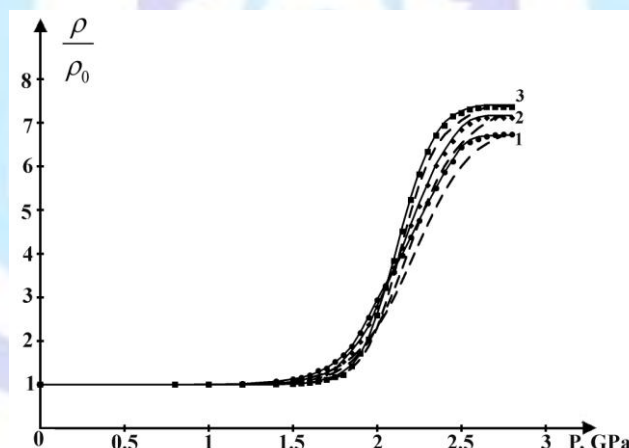

Fig 1: Dependence of piezoresistance for single crystals *n-Ge* on uniaxial pressure along the crystallographic direction [100] for different fixed temperatures: 1 – 180 K; 2 – 150 K; 3 – 110 K. Solid curves - theoretical calculations with taking into account nonequivalent intervalley scattering of electrons between *L₁* and *Δ₁* minima. Dashed curves - theoretical calculations without taking into account nonequivalent intervalley scattering of electrons between *L₁* and *Δ₁* minima.

Such uniaxial deformation leads to the simultaneous displacement upward at a scale of energies of four *L₁* minima and descend of two *Δ₁* minima [11]. The availability of a plateau for these dependencies indicates implementation of the (*L₁-Δ₁*) type of inversion of an absolute minimum for such magnitudes of uniaxial pressures and temperatures. As it can be seen from fig.1, magnitude of piezoresistance *n-Ge* (plateau of function $\rho_P / \rho_0 = f(P)$) decreases with the increasing of temperature. Temperature dependencies of resistivity for undeformed and uniaxially deformed along the crystallographic direction [100] under pressure *P=3 GPa* single crystals n-Ge are given at fig. 2. Inversion of (*L₁-Δ₁*) type of absolute minimum is realized in single crystals of germanium under such pressures. The obtained results show that resistivity of undeformed single crystals *n-Ge* (L₁ model of conduction band) is changed according to the law and for $\rho \sim T^{1.66}$, and for uniaxially deformed (*Δ₁* model of conduction band) as $\rho \sim T^{1.53}$. The given temperature dependencies explain the

decrease of piezoresistance n-Ge under the conditions of the inversion of (L_1-Δ_1) type of an absolute minimum with the increasing of temperature.
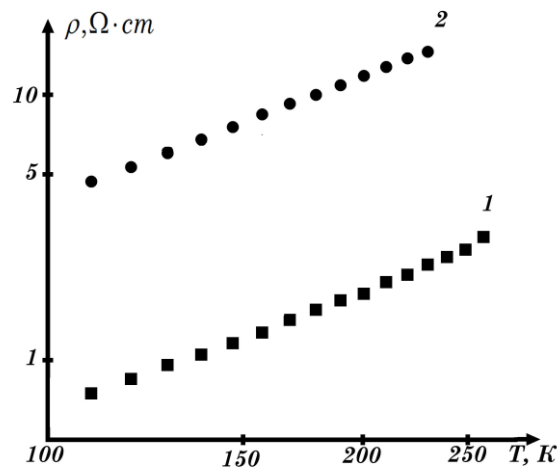

Fig 1: Temperature dependencies of resistivity for single crystals *n-Ge* : 1 – for undeformed single crystals *n-Ge* (L_1 model of conduction band); 2 – for uniaxially deformed under pressure *P=3 GPa* single crystals *n-Ge* (Δ_1 model of conduction band)

The given temperature dependencies of resistivity n-Ge are explained by the additional mechanism of scattering of electrons on optical and intervalley phonons in the model of L_1 and lack of this scattering mechanism in model of Δ_1. Intervalley scattering between the minima L_1 and Δ_1 should be taking into account along with the examined mechanisms of piezoresistance *n-Ge* (the same as in the case of hydrostatic pressure). On the basis of theory of the anisotropic scattering calculations for curves of piezoresistance *n-Ge* with consideration and without consideration of intervalley scattering between L_1 and Δ_1 minima have been done by us to determine the relative contribution of this scattering mechanism in piezoresistance *n-Ge*.

THE RESULTS OF THEORETICAL CALCULATIONS

Resistivity of uniaxially deformed along the crystallographic direction [100] single crystals *n-Ge* can be presented as:

$$\sigma = q(n_{L_1}\mu_{L_1} + n_{\Delta_1}\mu_{\Delta_1}),$$ (1)

where n_{L_1}, n_{Δ_1} , $\mu_{L_1}, \mu_{\Delta_1}$ - concentration and mobility of electrons for L_1 and Δ_1 minima correspondingly, *q* - electron charge.

For not degenerated electron gas

$$n_{L_1} = 2\left(\frac{2\pi m_{L_1} kT}{\hbar^2}\right)^{3/2} e^{\frac{E_F - E_{L_1}}{kT}}, n_{\Delta_1} = 2\left(\frac{2\pi m_{\Delta_1} kT}{\hbar^2}\right)^{3/2} e^{\frac{E_F - E_{\Delta_1}}{kT}}.$$ (2)

Then

$$\frac{n_{L_1}}{n_{\Delta_1}} = \left(\frac{m_{L_1}}{m_{\Delta_1}}\right)^{3/2} e^{\frac{\Delta E(P)}{kT}} = A,$$ (3)

where $\Delta E(P) = E_{\Delta_1} - E_{L_1}$, a E_{L_1}, E_{Δ_1} - energies of L_1 and Δ_1 minima in the strained crystal; m_{L_1} , m_{Δ_1} - effective mass for the density of states in these minima.

For undeformed single crystals of *n-Ge* energy gap between L_1 and Δ_1 is equal *0.18 eV* and decreases linearly from uniaxial pressure [12]. Then for the case of the deformed single crystals of *n-Ge* can be written:

$$\Delta E(P) = 0.18 - \beta P,$$ (4)

where $\beta = 8.97 \cdot 10^{-11} \frac{eV}{Pa}$ - baric coefficient for the change of magnitude of the energy gap between L_1 and Δ_1 minima

under uniaxial pressure along the crystallographic direction [100] [12].

Since the energy levels of admixture under the investigated temperatures are ionized completely, so is

$$n_{L_1} + n_{\Delta_1} = n = N_D .$$
(5)

Then, taking into account expressions (3) and (5), resistivity for uniaxially deformed single crystals *n-Ge* is

$$\rho = \frac{1}{\sigma} = \frac{A+1}{qN_D\left(A\mu_{L_1} + \mu_{\Delta_1}\right)} .$$
(6)

Isoenergetic surfaces for both L_1 and Δ_1 minima are ellipsoids of rotation. Then mobility of charge carriers in an arbitrary direction can be determined from the ratio [13]:

$$\mu = \mu_\perp \sin^2\theta + \mu_\parallel \cos^2\theta ,$$
(7)

where θ - angle between the examined direction and major axis of the ellipsoid; $\mu_\perp$ i $\mu_\parallel$ - mobility of charge carriers across and along the axis of the ellipsoid.

Then, according to (1), for the L_1 minimum

$$\mu^{L_1} = \frac{1}{3}\mu_\parallel^{L_1} + \frac{2}{3}\mu_\perp^{L_1} ,$$
(8)

for the Δ_1 – minimum, when *P//J//[100]*

$$\mu^{\Delta_1} = \mu_\parallel^{\Delta_1} .$$
(9)

Components for the tensor of mobility $\mu_\perp$ and $\mu_\parallel$ can be expressed through the tensor components of relaxation times and effective masses for the corresponding minimums:

$$\mu_\parallel^{L_1,\Delta_1} = \frac{q}{m_\parallel^{L_1,\Delta_1}} < \tau_\parallel^{L_1,\Delta_1} >, \mu_\perp^{L_1,\Delta_1} = \frac{q}{m_\perp^{L_1,\Delta_1}} < \tau_\perp^{L_1,\Delta_1} > .$$
(10)

On the basis of the theory of anisotropic scattering expressions for $\tau_\parallel^{L_1,\Delta_1}$ and $\tau_\perp^{L_1,\Delta_1}$ under conditions of scattering of electrons by admixture ions and acoustic phonons (intravalley scattering) will be as following [14]:

$$\tau_\parallel^{L_1,\Delta_1} = \frac{a_\parallel^{L_1,\Delta_1}}{\sqrt{k}T^{\frac{3}{2}}} \cdot \frac{x^{\frac{3}{2}}}{x^2 + b_0^{L_1,\Delta_1}} , \tau_\perp^{L_1,\Delta_1} = \frac{a_\perp^{L_1,\Delta_1}}{\sqrt{k}T^{\frac{3}{2}}} \cdot \frac{x^{\frac{3}{2}}}{x^2 + b_1^{L_1,\Delta_1}} .$$
(11)

(Necessary notations in expressions (11) are listed in the appendix).

Also necessary to take into account conduction bands for scattering of electrons on optical phonons, which frequencies correspond to temperature $T_{C1} = 430\ K$ (intravalley scattering) and intervalley scattering on acoustic phonons with a typical temperature $T_{C2} = 320\ K$ [15] for L_1 model of conduction band along with the scattering of electrons on the acoustic phonons and ions of admixture in *n-Ge*. Equivalent intervalley scattering on acoustic and optical phonons with characteristic temperatures $T_{C1} = 100\ K$ and $T_{C1} = 430\ K$ between the valleys, which are located on the same axis (g-scattering) [16] holds for two-valley Δ_1 model of conduction band single crystals n-Ge which has been formed by uniaxial pressure *P//[100]*. Role of the nonequivalent intervalley scattering will increase owing to reduction of the energy gap between L_1 and Δ_1 minima under uniaxial pressure. Nonequivalent $L_1 \leftrightarrow \Delta_1$ intervalley scattering of electrons is stipulated by their interaction with acoustic phonons with the characteristic temperature $T_{C2}=320\ K$ [16]. Scattering of electrons on optical and intervalley phonons can be described by the scalar time of relaxation τ_{ij} [16]:

$$\frac{1}{\tau_{ij}} = a_{ij}\phi_i ,$$
(12)

where

$$a_{ij} = \frac{\Xi_{ij}^2 \left(m_d^j\right)^{3/2}}{\sqrt{2}\pi\rho\hbar^2 \left(kT_{Cj}\right)^{1/2}} \left(\frac{T}{T_{Cj}}\right)^{1/2}, \quad \phi_i(x) = \frac{1}{e^{\frac{T_{Cj}}{T}}-1}\left[\left(x+\Delta E^*(P)+\frac{T_{Cj}}{T}\right)^{1/2} + e^{\frac{T_{Cj}}{T}}\theta(x;\frac{T_{Cj}}{T})\left(x+\Delta E^*(P)-\frac{T_{Cj}}{T}\right)^{1/2}\right],$$

m_d^j - combined mass of the density of states for j - minimum; Ξ_{ij} - constant of intervalley or optical potential of deformation; ρ - density of crystal; T_{Cj} - temperature of j - intervalley or optical phonon; $x = \frac{\varepsilon}{kT}$ - nondimensional energy of electron; $\theta(x;\frac{T_{Cj}}{T})$ - step function; $\Delta E^*(P) = \frac{\Delta E(P)}{kT}$.

For the equivalent intervalley scattering [16]

$$m_d^j = \left(m_{\parallel j}m_{\perp j}^2\right)^{1/3}\left(Z_j - 1\right), \tag{13}$$

and for the nonequivalent scattering

$$m_d^j = \left(m_{\parallel j}m_{\perp j}^2\right)^{1/3} Z_j, \tag{14}$$

where $m_{\parallel j}$, $m_{\perp j}$ - longitudinal and transverse component of tensor effective mass for electrons, which are in ellipsoid of j - type; Z_j - number of the equivalent ellipsoids of j - type conduction band.

For intravalley scattering of electrons on the optical phonons

$$m_d^j = \left(m_{\parallel j}m_{\perp j}^2\right)^{1/3} Z_j^{2/3}. \tag{15}$$

Then for the most general case for scattering of electrons on the acoustic phonons, ions of admixture, optical and intervalley phonons expressions for the tensor components of relaxation times for L_1 and Δ_1 minima will be as following:

$$\frac{1}{\tau_{\parallel}^{L_1}} = \frac{1}{\tau_{\parallel}} + \frac{1}{\tau_1} + \frac{1}{\tau_2} + \frac{1}{\tau_{12}} + \frac{1}{\tau_{21}}, \quad \frac{1}{\tau_{\perp}^{L_1}} = \frac{1}{\tau_{\perp}} + \frac{1}{\tau_1} + \frac{1}{\tau_2} + \frac{1}{\tau_{12}} + \frac{1}{\tau_{21}}, \tag{16}$$

$$\frac{1}{\tau_{\parallel}^{\Delta_1}} = \frac{1}{\tau_{\parallel}} + \frac{1}{\tau_3} + \frac{1}{\tau_4} + \frac{1}{\tau_{12}} + \frac{1}{\tau_{21}}, \tag{17}$$

where $\tau_{\parallel}^{L_1,\Delta_1}$, $\tau_{\perp}^{L_1,\Delta_1}$ - longitudinal and transverse components for tensor of relaxation times in case of scattering by acoustic phonons (intravalley scattering) and ions of admixture for L_1 and Δ_1 minima; τ_1 , τ_2 - times of relaxation for intervalley scattering on acoustic phonons with characteristic temperature T_{C1}=320 K and scattering at optical phonons with characteristic temperature T_{C2}=430 K (intravalley scattering) for L_1 minima; τ_3 , τ_4 - times of relaxation for intervalley scattering of electrons (g - scattering) at acoustic and optical phonons with characteristic temperatures T_{C1}=100 K та T_{C2}=430 K for Δ_1 minima; τ_{12} , τ_{21} - times of relaxation for nonequivalent $L_1 \rightarrow \Delta_1$ and $\Delta_1 \rightarrow L_1$ intervalley scattering of electrons at acoustic phonons with characteristic temperature T_C=320 K.

For a nondegenerate electron gas

$$\left\langle \tau_{\parallel}^{L_1,\Delta_1} \right\rangle = \frac{4}{3\sqrt{\pi}}\int_0^\infty dx x^{\frac{3}{2}} e^{-x}\tau_{\parallel}^{L_1,\Delta_1}, \quad \left\langle \tau_{\perp}^{L_1,\Delta_1} \right\rangle = \frac{4}{3\sqrt{\pi}}\int_0^\infty dx x^{\frac{3}{2}} e^{-x}\tau_{\perp}^{L_1,\Delta_1}. \tag{18}$$

The mobility of electrons for L_1 and Δ_1 minima can be found taking into consideration the expressions (8–18). This will allow (on the basis of the expressions (3-6)) to find the dependence of resistivity *n-Ge* from uniaxial pressure along the crystallographic direction [100]. Constants of optical and intervalley deformation potential, components for tensor of the acoustic deformation potential for intravalley scattering, effective mass for the density of states and tensor components of the effective mass for L_1 and Δ_1 minima are necessary for this process. A significant number of the given parameters had been found by us in works [12, 15, 17]. The necessary parameters of L_1 and Δ_1 minima for calculation are presented in the table 1.

Table 1. Parameters of L_1 and Δ_1 minima for the conduction band of germanium.

Parameters		Conduction band of germanium	
Name	**Symbols**	L_1 minima	Δ_1 minima
Components for tensor of the effective mass	$m_{\parallel}$	$1.58m_0$ [18]	$1.65m_0$ [17]
	$m_{\perp}$	$0.082m_0$ [18]	$0.32m_0$ [17]
Effective mass for the density of states	m_{L_1,Δ_1}	$0.55m_0$ [18]	$0.88m_0$ [17]
Components for tensor of the acoustic deformation potential for intravalley scattering	Ξ_u (eV)	16.4 [18]	11.82 [12]
	Ξ_d (eV)	-6.4 [18]	-1.29 [12]
Constant for optical deformation potential T_C=430 K	Ξ_{430} (eV/cm)	$4 \cdot 10^8$ [15]	
Constant for intervalley deformation potential T_C=320 K	Ξ_{320} (eV/cm)	$1.4 \cdot 10^8$ [15]	
Constant for intervalley deformation potential for nonequivalent $L_1 \leftrightarrow \Delta_1$ scattering T_C=320 K	Ξ_{320} (eV/cm)	$5.5 \cdot 10^8$ [16]	
Constants for intervalley deformation potential for g –scattering T_{C1}=100 K T_{C2}=430 K	Ξ_{100} (eV/cm)		$7.89 \cdot 10^7$ [16]
	Ξ_{430} (eV/cm)		$1.57 \cdot 10^8$ [16]

Results of theoretical calculations of the piezoresistance *n-Ge* with taking into account (solid curves) and without taking into account (dashed curves) of the nonequivalent intervalley scattering between L_1 and Δ_1 minima are presented in fig. 1.

CONCLUSIONS

Characteristic features of piezoresistance *n-Ge* (when (L_1-Δ_1) model of conduction band is implemented) can be described only taking into account the given mechanism of scattering. Such conclusions have been done by us after comparison of these curves with the relevant experimental results. Presence of the significant piezoresistance ρ_{∞}/ρ_0 under uniaxial pressures *P>2.7 GPa* is explained by the increase in the effective mass and a decrease in the relaxation time for electrons at the expense of the inversion of (L_1-Δ_1) type of an absolute minimum in *n-Ge*. Reduction of the magnitude piezoresistance ρ_{∞}/ρ_0 *n-Ge* with the increasing temperature (fig.1, reduction of the magnitude of the plateau curves 1-3) is associated with "turning-off" at the expense of the uniaxial deformation of mechanism for scattering of electrons on intervalley and optical phonons during the transition from L_1 to Δ_1 model of the conduction band *n-Ge*.

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APPENDIX

$$a_{\parallel} = \frac{\pi C_{11} \hbar^4}{k \Xi_d^2 \sqrt{2 m_{\parallel} m_{\perp}^2}} \cdot \frac{1}{\Phi_{0a}}, \, a_{\perp} = \frac{\pi C_{11} \hbar^4}{k \Xi_d^2 \sqrt{2 m_{\parallel} m_{\perp}^2}} \cdot \frac{1}{\Phi_{1a}}, \tag{1}$$

$$b_0 = \frac{a_{\parallel} \cdot \Phi_{0i}}{\sqrt{kT}^{\frac{3}{2}} \tau_{0i}(kT)}, \, b_1 = \frac{a_{\perp} \cdot \Phi_{1i}}{\sqrt{kT}^{\frac{3}{2}} \tau_{0i}(kT)}, \tag{2}$$

$$\tau_{0i}(kT) = \frac{\sqrt{2} m_{\perp} \varepsilon^2 (kT)^{\frac{3}{2}}}{\pi N e^4 \sqrt{m_{\parallel}}}, \tag{3}$$

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

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

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

(6)

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

where $\alpha = arctg\,\beta$, $\beta^2 = \dfrac{m_\parallel - m_\perp}{m_\perp}$, $\gamma = \sqrt{\dfrac{\pi\,\hbar^2 e^2 n}{2m_\parallel \varepsilon\varepsilon_0 kT}}$,

$L(\alpha) = -\int\limits_0^\alpha \ln\cos\phi\,d\phi -$ Lobachevskyi function,

n – concentration of electrons.

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