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**THERMOEMF IN L_1 - Δ_1 MODEL
OF GERMANIUM UNDER HIGH
HYDROSTATIC PRESSURE**

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- *At high hydrostatic pressure an electron transfer takes place from four L_1 valleys to six equivalent Δ_1 valleys and band structure of n-type Germanium is converted into one, similar to the n-type Silicon structure. The deformation potentials of L_1 - and Δ_1 valleys and their pressure behavior has been analyzed under low temperature $T = 78$ K and room temperature $T = 300$ K. The theory of anisotropic scattering has been used to calculate thermoEMF. The intraband scattering of electrons by acoustic phonons and impurity ions and interband nonequivalent electron scattering between L_1 - and Δ_1 valleys as well as interband equivalent f - and g - scattering between Δ_1 -valleys have been considered.*

Introduction

The energetic structure of the conduction band of *Ge* is well known [1–3] and at the atmospheric pressure the four lowest L_1 conduction band valleys are occupied by electrons. However, with increasing hydrostatic pressure, the energy of four L_1 valleys increases with respect to the bottom of conduction band in undeformed crystal. The Δ_1 minima have a negative pressure coefficient and shift down in energetic scale [1-3]. Only four L_1 valleys always were considered in case of undeformed single crystals or in case of their relatively small deformation (L_1 model of Germanium) [4–6]. Under strong elastic pressure the Δ_1 valleys must be involved in consideration ($L_1 - \Delta_1$ model of Germanium) [1–3, 7–9, 13, 14]. Under a determined pressure P_0 the position of two groups of valleys becomes the same on energetic scale. In case of pressure gradually increases, the band crossover of L_1 and Δ_1 valleys takes place, i.e. the Δ_1 valleys will be localized lower on the energetic scale relatively the L_1 valleys. Under the sufficiently high pressure practically all electrons will be localized in Δ_1 valleys (Δ_1 model of Germanium) and, consequently, the structure of the band becomes similar to the Silicon one under atmospheric pressure. Under these conditions the Δ_1 valleys become accessible for direct experimental electrical measurement [2, 3], and consequently theoretical considerations of transport phenomena are not purely artificial. In this paper we try to analyze the thermoEMF under high hydrostatic pressure.

Occupation numbers and chemical potential

In the assumption about no degeneration of electron gas the equilibrium distribution of electrons in L_1 and Δ_1 valleys may be written as [5, 6]

$$\bar{f}_k^{(i)} = \exp(\bar{\mu}^* - E_{L_1}^{(i)*} - \varepsilon_k^{(i)*}), \bar{f}_k^{(j)} = \exp(\bar{\mu}^* - \Delta E_0^* - E_{\Delta_1}^{(j)*} - \varepsilon_k^{(j)*}), \quad (1)$$

here $\bar{\mu}^* = \bar{\mu}/kT$ is reduced chemical potential in deformed single crystal, $E_{L_1, \Delta_1}^{(i,j)}$ are reduced

deformation potentials of L_1 - and Δ_1 -valleys, $\Delta E_0^* = \Delta E_0/kT$ is reduced distance on energy scale between L_1 - and Δ_1 - minima in undeformed single crystal.

The total number of electrons in each L_1 - and Δ_1 -valleys is respectively

$$N_{L_1}^{(i)} = \frac{2}{(2\pi)^3} \int \bar{f}_{\vec{k}}^{(i)} d\vec{k} = 2 \frac{(2\pi kT)^{\frac{3}{2}} \left[(m_{\perp}^{L_1})^2 m_{\parallel}^{L_1} \right]^{\frac{1}{2}}}{(2\pi\hbar)^3} \cdot \exp(\bar{\mu}^* - E_{L_1}^{(i)*}),$$

$$N_{\Delta_1}^{(j)} = 2 \frac{(2\pi kT)^{\frac{3}{2}} \left[(m_{\perp}^{\Delta_1})^2 m_{\parallel}^{\Delta_1} \right]^{\frac{1}{2}}}{(2\pi\hbar)^3} \cdot \exp(\bar{\mu}^* - E_{\Delta_1}^{(j)*} - \Delta E_0^*). \quad (2)$$

It is easy to find from (2) the number of electrons in each valley of undeformed crystal N_{L_1, Δ_1}^0 by substitution $E_{L_1, \Delta_1}^{(i,j)} = 0$, $\bar{\mu}^* \rightarrow \mu^*$, where μ^* is chemical potential of undeformed crystal.

We note that to find the deformation potentials that we have in (1)–(2) is necessary to use the deformation potential theory for cubic crystals [5, 6, 10]. The deformation potential for i - valley, as follows from this theory, at the coordinate system connected with main axis of effective mass tensor is

$$E_i = C_1(\varepsilon_{11}^{(i)} + \varepsilon_{22}^{(i)} + \varepsilon_{33}^{(i)}) + C_2\varepsilon_{33}^{(i)},$$

where $C_1^{(i)}$ and $C_2^{(i)}$ are deformations potential constants, $\varepsilon_{ll}^{(i)}$ are the components of deformation tensor of i - valley. Usually all deformation potentials and, consequently, all deformation tensor components must be expressed at the same laboratory coordinate systems connected with the crystallographic axis [100], [010], [001]. It is easy to find their using the Hook's law in form

$$\varepsilon_{ik} = \sum_{l,m} S'_{iklm} U_{lm},$$

where U_{lm} are the elastic stress tensor components, in case of hydrostatic pressure at the laboratory coordinate system the stress tensor has three equal diagonal components, $U_{lm} = P\delta_{lm}$, $P < 0$ corresponds to compression; S'_{iklm} are the elastic compliances tensor, the components of this tensor usually are known in crystallographic axes [11]. In our case crystallographic coordinate system coincide with laboratory one.

The deformation potentials after converting deformation tensor components of each valley to laboratory coordinate system will have the form

$$E_{L_1}^{(1-4)} = 3\left(C_1^{L_1} + \frac{1}{3}C_2^{L_1}\right)(S_{11} + 2S_{12})P,$$

$$E_{\Delta_1}^{(1-6)} = 3\left(C_1^{\Delta_1} + \frac{1}{3}C_2^{\Delta_1}\right)(S_{11} + 2S_{12})P. \quad (3)$$

Here S_{ik} are Voigt's matrix designation of elastic compliance tensor's components: $S_{11} = S_{1111}$; $S_{12} = S_{1122}$. The all deformation potentials for L_1 - valleys are equal and positives, because $C_1^{L_1} + \frac{1}{3}C_2^{L_1} < 0$ [5], $S_{11} + 2S_{12} > 0$ and $P < 0$ for compression. This means that four L_1 - valleys shifts up in energetic scale with pressure P increases. At the same time the all deformation potentials for Δ_1 -valleys are equal and will be negatives and will shift down in energetic scale with pressure P increases accordingly experimental data [1–3] if $C_1^{\Delta_1} + \frac{1}{3}C_2^{\Delta_1} > 0$.

Using the electroneutrality equation for undeformed ($4N_{L_1}^0 + 6N_{\Delta_1}^0 = N_0$) and deformed

($4N_{L_1} + 6N_{\Delta_1} = N_0$) crystal it is easy obtain relation between chemical potential in deformed ($\bar{\mu}^*$) and undeformed (μ^*) crystal

$$e^{\bar{\mu}^*} = \left[4 + 6 \left(m_N^{\Delta_1} / m_N^{L_1} \right)^{3/2} e^{-\Delta E_0^*} \right] \left[4 + 6 \left(m_N^{\Delta_1} / m_N^{L_1} \right)^{3/2} e^{E_{L_1}^* - E_{\Delta_1}^* - \Delta E_0^*} \right]^{-1} e^{\mu^*} \quad (4)$$

and can be derived the expressions for the relative numbers of valley occupation with electrons $n_r^{(i)} = N_r^{(i)} / N_0$

$$n_{L_1} = \left\{ 4 + 6 \left(\frac{m_N^{\Delta_1}}{m_N^{L_1}} \right)^{3/2} \cdot \exp(E_{L_1}^* - E_{\Delta_1}^* - \Delta E_0^*) \right\}^{-1},$$

$$n_{\Delta_1} = \left\{ 4 \left(\frac{m_N^{L_1}}{m_N^{\Delta_1}} \right)^{3/2} \cdot e^{\Delta E_0^* + E_{\Delta_1}^* - E_{L_1}^*} + 6 \right\}^{-1}. \quad (5)$$

Here $m_N^{L_1, \Delta_1} = \left[\left(m_{\perp}^{L_1, \Delta_1} \right)^2 m_{\parallel}^{L_1, \Delta_1} \right]^{1/3}$ is the effective mass of density of states in L_1 and Δ_1 valleys.

In undeformed crystal $P = 0$, $n_{L_1} = 0.25$, $n_{\Delta_1} \approx 0$. In case of high pressure $P > P_0$ practically all electrons are localized in Δ_1 -valleys, $n_{L_1} \approx 0$, $n_{\Delta_1} = 1/6$. At the band crossover pressure $P = P_0$ all ten valleys (L_1 - and Δ_1 -valleys) are energetically equivalent, i.e. $E_{L_1} = \Delta E_0 + E_{\Delta_1}$ and from (5) follow $n_{L_1} / n_{\Delta_1} = \left(m_N^{L_1} / m_N^{\Delta_1} \right)^{3/2}$, that mean that there are equal number of electrons in each type of valleys only if the effective masses of density of states will be equal in each type of valleys.

From (4) and (5) it is possible to determine the explicit expression for chemical potential in deformed and undeformed crystals and show it in two different but equivalent forms:

$$\bar{\mu}^* = \mu^* + E_{L_1}^* + \ln(n_{L_1} / n_0),$$

$$\bar{\mu}^* = \mu^* + E_{\Delta_1}^* + \Delta E_0^* + \ln(n_{\Delta_1} / n_0) + (3/2) \ln(m_N^{L_1} / m_N^{\Delta_1}). \quad (6)$$

specifying that $n_0 = \left[4 + 6 \left(m_N^{L_1} / m_N^{\Delta_1} \right)^{3/2} e^{-\Delta E_0^*} \right]^{-1}$.

The chemical potential of the undeformed crystal can be calculated in a usual manner.

Diffusion thermoEMF

First of all we shall discuss briefly main scattering mechanisms of electrons in our model. We shall limit our consideration to phonon and impurity ion scattering processes within the L_1 and Δ_1 valleys. In the L_1 and Δ_1 valleys the electrons are subject to the following scattering processes: intravalley acoustic and impurity ion scattering and also non-equivalent intervalley scattering between L_1 and Δ_1 valleys. Furthermore in Δ_1 valleys electrons are subject to the equivalent intervalley scattering between valleys lying on the same cube axis (g -scattering) and equivalent intervalley scattering between valley lying on the perpendicular cube axis (f -scattering).

We suppose that all indicated scattering processes may be described through appropriate relaxation times and Mattisens' rule is valid in this case. The intravalley acoustic phonon scattering as well as intravalley ionized impurity scattering in linear approximation may be described using diagonal relaxation time tensor with two components, which can be seen in detail in [4–9]. Intervalley scattering of electron caused by interaction with acoustic and optic phonons with frequencies corresponding the temperatures $T_{c1} = 320$ K (non-equivalent intervalley scattering between L_1 and Δ_1

valleys and equivalent intervalley f -scattering), $T_{c_2} = 430$ K and $T_{c_3} = 100$ K (equivalent intervalley g -scattering) may be described by scalar relaxation time [1, 4–9, 12], which we can generalize, considering the kinetic of valleys described above under high hydrostatic pressure. All kinetic integrals will have the same analytic form as in [8].

It has been known [4-6], the thermoEMF tensor is defined by relation

$$\alpha_{ik} = \rho_{il} b_{lk} . \quad (7)$$

Beforehand we should consider the tensor of specific resistivity. In order to determine it we should start by finding the tensor of specific electrical conductivity. For single n - Ge crystal in the case of hydrostatic pressure it can be calculated in the following manner

$$\sigma_{ik} = \sum_{r=1}^4 \sigma_{ik}^{(r)L} + \sum_{r=1}^6 \sigma_{ik}^{(r)\Delta} . \quad (8)$$

In this expression $\sigma_{ik}^{(r)L,\Delta}$ are components of electrical conductivity tensor for L_1 - and Δ_1 -valleys written in the laboratory coordinate system. In the main axis of the mass tensor of i -th valley, the tensor of effective specific electrical conductivity of electrons of this valley has two different from zero components [5–8], which after being averaged by energies look as following:

$$\sigma_{11=22,33}^{(i)} = \sigma_{\perp,\parallel}^{(i)} = \frac{4}{3\sqrt{\pi}} \frac{N_0' e^2}{T\sqrt{kT}} \frac{a_{\perp,\parallel}^{(i)}}{m_{\perp}^{(i)}} J_{\perp,\parallel}^{(i)}(3) . \quad (9)$$

All designation are the same as in [8]. Tensor of specific electrical conductivity of crystal is found, as usual, by transformation of tensor component of electrical conductivity tensor of each valley to laboratorial coordinate system, following the addition by all L_1 and Δ_1 valleys using (8). As the result of some non-complicated calculations we have:

$$\sigma_{\alpha\beta} = \frac{8}{9\sqrt{\pi}} \cdot \frac{N_0 e^2}{T\sqrt{kT}} \cdot \left\{ 2n_{L_1} \left(2 \frac{a_{\perp}^{L_1}}{a_{\parallel}^{L_1}} J_{\perp}^{L_1} + \frac{a_{\parallel}^{L_1}}{m_{\parallel}^{L_1}} J_{\parallel}^{L_1} \right) + 3n_{\Delta_1} \left(2 \frac{a_{\perp}^{\Delta_1}}{m_{\perp}^{\Delta_1}} J_{\perp}^{\Delta_1} + \frac{a_{\parallel}^{\Delta_1}}{m_{\parallel}^{\Delta_1}} J_{\parallel}^{\Delta_1} \right) \right\} \delta_{\alpha\beta} . \quad (10)$$

The last formula can be rewritten in compact form introducing the effective anisotropy scattering parameter

$$K_{L_1,\Delta_1} = \frac{m_{\parallel}^{L_1,\Delta_1} a_{\perp}^{L_1,\Delta_1}}{m_{\perp}^{L_1,\Delta_1} a_{\parallel}^{L_1,\Delta_1}} \cdot \frac{J_{\perp}^{L_1,\Delta_1}(3)}{J_{\parallel}^{L_1,\Delta_1}(3)} = K_a^{L_1,\Delta_1} \cdot \frac{J_{\perp}^{L_1,\Delta_1}(3)}{J_{\parallel}^{L_1,\Delta_1}(3)} , \quad (11)$$

and taking into account (9). In this case

$$\sigma_{\alpha\beta} = \left\{ 4n_{L_1} \sigma_{\perp}^{L_1} \frac{2K_{L_1} + 1}{3K_{L_1}} + 6n_{\Delta_1} \sigma_{\perp}^{\Delta_1} \frac{2K_{\Delta_1} + 1}{3K_{\Delta_1}} \right\} \delta_{\alpha\beta} . \quad (12)$$

From experiments with pure crystals it is known that under low temperature $T = 78$ K $K_{L_1} = 16.4$ and $K_{\Delta_1} = 4.4$ [5, 13, 14].

As well known, the hydrostatic pressure doesn't change the symmetry of the crystal and in cubic crystals the tensor of electrical conductivity is a scalar. This fact is reflected by the last formula. It is obvious that resistivity tensor components can be calculated using a formula:

$$\rho_{ii} = 1/\sigma_{ii} . \quad (13)$$

Let us note that the dependence on the pressure in (10), (12) comes via occupation numbers and integrals, where relaxation time of non-equivalent “interband” scattering depends on pressure.

For a separately taken “ i ” valley with availability of deformation the symmetry of $b_{ik}^{e,(i)}$ tensor coincides with symmetry of $\sigma_{ik}^{(i)}$ tensor because [6]

$$b_{ik}^{e,(i)} = -\left\langle \sigma_{ik}^{(i)}(\bar{x}, P) \cdot \alpha^{e,(i)}(\bar{x}, P) \right\rangle. \quad (14)$$

Here $\sigma_{ik}^{(i)}(\bar{x}, P)$ – electrical conductivity of the i -th valley, caused by the group of electrons with reduced energy \bar{x} , scalar $\alpha^{e,(i)}(\bar{x}, P)$ is electron thermoEMF of the i -th valley, determined by the diffusion of the group of electrons with reduced energy \bar{x} and available of deformation [6]: $\alpha^{e,(i)}(\bar{x}, P) = (k/e)(\bar{x} - \bar{\mu}^*)$.

Components of the tensor $b_{ik}^{e,(i)}$ of a i -th valley, take the following form after averaging by energies:

$$b_{11=22,33}^{e,(i)} = b_{\perp,\parallel}^{e,(i)} = -\frac{k}{e} \frac{4}{3\sqrt{\pi}} \frac{N_0' e^2}{T\sqrt{kT}} n_i \frac{a_{\perp,\parallel}^{(i)}}{m_{\perp,\parallel}^{(i)}} \left[J_{\perp,\parallel}^{(i)}(4) - \bar{\mu}^* J_{\perp,\parallel}^{(i)}(3) \right]. \quad (15)$$

Using the effective anisotropy scattering parameter (14) and introducing the denote $\xi_{\perp,\parallel}^{(i)} = J_{\perp,\parallel}^{(i)}(4)/J_{\perp,\parallel}^{(i)}(3)$, the expression (15) becomes

$$b_{\perp}^{e,(i)} = -\frac{k}{e} n_i \sigma_{\perp}^{(i)} (\xi_{\perp}^{(i)} - \bar{\mu}^*), \quad b_{\parallel}^{e,(i)} = -\frac{k}{e} n_i \sigma_{\parallel}^{(i)} \frac{1}{K_i} (\xi_{\parallel}^{(i)} - \bar{\mu}^*). \quad (16)$$

After transforming the component of the $b_{ik}^{e,(i)}$ tensor of each valley into laboratorial coordinate system and summing by all groups of equivalent valleys for b_{ik}^e tensor we have:

$$b_{11}^e = b_{22}^e = b_{33}^e = \frac{4}{3} (2b_{\perp}^{L_1} + b_{\parallel}^{L_1}) + 2(2b_{\perp}^{\Delta_1} + b_{\parallel}^{\Delta_1}). \quad (17)$$

Taking into consideration (11), (15) and introducing the denotes

$$r_{L_1, \Delta_1} = \frac{J_{\parallel}^{L_1, \Delta_1}(4) J_{\perp}^{L_1, \Delta_1}(3)}{J_{\perp}^{L_1, \Delta_1}(4) J_{\parallel}^{L_1, \Delta_1}(3)},$$

the expression (16) becomes

$$b_{ii}^{(e)} = -\frac{k}{e} \left[4n_{L_1} \sigma_{\perp}^{L_1} \left(\xi_{\perp}^{L_1} \frac{2K_{L_1} + r_{L_1}}{3K_{L_1}} - \bar{\mu}^* \frac{2K_{L_1} + 1}{3K_{L_1}} \right) + 6n_{\Delta_1} \sigma_{\perp}^{\Delta_1} \left(\xi_{\perp}^{\Delta_1} \frac{2K_{\Delta_1} + r_{\Delta_1}}{3K_{\Delta_1}} - \bar{\mu}^* \frac{2K_{\Delta_1} + 1}{3K_{\Delta_1}} \right) \right] \delta_{ii}. \quad (18)$$

It is evidently, that thermoEMF will be scalar too.

The diffusion thermoEMF in the explicit form may be calculate without any difficulties using (7), (12) and (13) and finally we obtain

$$\alpha_{ii}^{(e)} = \frac{k}{e} \frac{4n_{L_1} \sigma_{\perp}^{L_1} \left(\xi_{\perp}^{L_1} \frac{2K_{L_1} + r_{L_1}}{3K_{L_1}} - \bar{\mu}^* \frac{2K_{L_1} + 1}{3K_{L_1}} \right) + 6n_{\Delta_1} \sigma_{\perp}^{\Delta_1} \left(\xi_{\perp}^{\Delta_1} \frac{2K_{\Delta_1} + r_{\Delta_1}}{3K_{\Delta_1}} - \bar{\mu}^* \frac{2K_{\Delta_1} + 1}{3K_{\Delta_1}} \right)}{4n_{L_1} \sigma_{\perp}^{L_1} \frac{2K_{L_1} + 1}{3K_{L_1}} + 6n_{\Delta_1} \sigma_{\perp}^{\Delta_1} \frac{2K_{\Delta_1} + 1}{3K_{\Delta_1}}} \delta_{ii}. \quad (19)$$

In case of no deformed crystal $n_{\Delta_1} \approx 0$ and from the last expression follows

$$\alpha_{ii}^{(e)} = \frac{k}{e} \left(\xi_{\perp}^{L_1} \frac{2K_{L_1} + r_{L_1}}{2K_{L_1} + 1} - \bar{\mu}^* \right) \delta_{ii}. \quad (20)$$

At the presence only intraband acoustic scattering the formula (20) results $\alpha_{ii}^{(e)} = \frac{k}{e} (2 - \bar{\mu}^*) \delta_{ii}$.

In case of strong elastic deformation, after band crossover, practically all electrons are localized in Δ_1 -valleys ($n_{L_1} \approx 0$, $n_{\Delta_1} = 1/6$) and formula (20) are valid with change index $L_1 \rightarrow \Delta_1$.

Phonon drag thermoEMF

It is known [4, 6, 8] that the component of the kinetic tensor $b_{ik}^{f,(i)}$ of i -th valley caused by phonon drag of electrons can be defined as:

$$b_{ik}^{f,(i)} = -\left\langle \sigma_{il}^{(i)}(x) \alpha_{lk}^{f,(i)}(x) \right\rangle. \quad (21)$$

Here $\alpha_{lk}^{f,(i)}(x)$ is thermoEMF's drag tensor, caused by group of electrons drag with reduced energy x by long-waved phonons of all polarizations. As has been shown in [6], for the biaxial ellipsoidal isoenergetic surface, the tensor $\alpha_{lk}^{f,(i)}(x)$ must contain the symmetry of energetic minima, i.e. tensor $\alpha_{lk}^{f,(i)}(x)$ have two independent components:

$$\alpha_{\perp}^f(x) = (k/e) f_{\perp}(x), \quad \alpha_{\parallel}^f(x) = (k/e) (m_{\parallel} / m_{\perp}) f_{\parallel}(x), \quad (22)$$

$$f_{\perp}(x) = \sum_j A_{n_j} \beta_{n_j} x^{n_j-1/2} I_{\perp, n_j}, \quad f_{\parallel}(x) = \sum_j A_{n_j} \beta_{n_j} x^{n_j-1/2} I_{\parallel, n_j}. \quad (23)$$

In the above expressions the addition is done by polarization of phonons, A_{n_j} - constant derived from comparison of experimental data and theoretical calculations, the method used to obtain them was described in [15, 16], constants β_{n_j} and $I_{\perp, \parallel, n_j}$ integrals depend on the characteristics of the energy valley and crystal itself and are shown in explicit form in [6], parameter n_j was found in [14, 15] and for germanium $n_l = 0.25$, $n_t = 0.5$.

Introducing the designations [6]

$$\alpha_{\perp, L_1, \Delta_1}^{(j)}(T) = (k/e) A_{n_j} \beta_{n_j, L_1, \Delta_1} I_{\perp, n_j}^{L_1, \Delta_1}, \quad (24)$$

$$\alpha_{\parallel, L_1, \Delta_1}^{(j)}(T) = (k/e) (m_{\parallel}^{L_1, \Delta_1} / m_{\perp}^{L_1, \Delta_1}) A_{n_j} \beta_{n_j, L_1, \Delta_1} I_{\parallel, n_j}^{L_1, \Delta_1} \quad (25)$$

and averaging by energy of electrons, for kinetic tensor components in coordinate system related with valley's main tensor mass axils, we obtain:

$$b_{11,33}^{f,(i)} = b_{\perp, \parallel}^{f,(i)} = \frac{4}{3\sqrt{\pi}} \frac{N_0' e^2}{T \sqrt{kT}} n_i \frac{a_{\perp, \parallel}^{(i)}}{m_{\perp, \parallel}^{(i)}} \alpha_{\perp, \parallel}^{(j,i)}(T) J_{\perp, \parallel}^{(i)}(5/2 + n_j). \quad (26)$$

For L_1 and Δ_1 valleys in correspondent multipliers, specific indexes should be introduced which indicate the type of a valley.

After transformation of the kinetic tensor's components $b_{\perp, \parallel}^{f,(i)}$ of each valley to laboratorial coordinate system and addition by all groups of equivalent valleys, it becomes not complex to get the expression for the components of the kinetic tensor of crystal. In order to simplify the expression that was obtained it would be comfortable to use the following designation:

$$\alpha_{\perp, \parallel}^f = \sum_j \alpha_{\perp, \parallel}^{(j)}(T) \frac{J_{\perp, \parallel}(5/2 + n_j)}{J_{\perp, \parallel}(3)}, \quad \bar{M} = \frac{\alpha_{\parallel}^f}{\alpha_{\perp}^f}, \quad (27)$$

where $\alpha_{\perp, \parallel}^f$ – transversal or longitudinal thermoEMF drag tensor components, conditioned by the drag of electrons belonging to one valley, \bar{M} – averaged thermoEMF drag's anisotropic

parameter. Let us underline that in the above designations all the magnitudes are related to a specific valley groups (L_1 or Δ_1) and later corresponding indexation will be attributed.

Using (12), for the component of the kinetic tensor \hat{b}^f of crystal in laboratorial coordinate system the following could be received:

$$b_{11}^f = b_{33}^f = 4n_{L_1} \sigma_{\perp}^{L_1} \alpha_{\perp, L_1}^f \frac{2K_{L_1} + \bar{M}_{L_1}}{3K_{L_1}} + 6n_{\Delta_1} \sigma_{\perp}^{\Delta_1} \alpha_{\perp, \Delta_1}^f \frac{2K_{\Delta_1} + \bar{M}_{\Delta_1}}{3K_{\Delta_1}}. \quad (28)$$

It is not difficult to obtain analytical relations for the thermoEMF drag tensor, considering all L_1 and Δ_1 valleys, since $\alpha_{ii}^f = b_{ii}^f / \sigma_{ii}$.

$$\alpha_{ii}^f = \frac{4n_{L_1} \sigma_{\perp}^{L_1} \alpha_{\perp, L_1}^f \frac{2K_{L_1} + \bar{M}_{L_1}}{3K_{L_1}} + 6n_{\Delta_1} \sigma_{\perp}^{\Delta_1} \alpha_{\perp, \Delta_1}^f \frac{2K_{\Delta_1} + \bar{M}_{\Delta_1}}{3K_{\Delta_1}}}{4n_{L_1} \sigma_{\perp}^{L_1} \frac{2K_{L_1} + 1}{3K_{L_1}} + 6n_{\Delta_1} \sigma_{\perp}^{\Delta_1} \frac{2K_{\Delta_1} + 1}{3K_{\Delta_1}}} \delta_{ii}, \quad (29)$$

i.e. α^f , as well as α^e , degenerates into the scalar due to cubic symmetry of crystal.

The relations (29) allow us to consider easily some particular cases.

For no deformed crystal the contribution of the Δ_1 valleys may be neglected (as it is obvious) and we can obtain a well-known formula for phonon drag thermoEMF of the undeformed n -Ge:

$$\alpha_{11}^f = \alpha_{33}^f = \alpha_{\perp, L_1}^f \frac{2K_{L_1} + \bar{M}_{L_1}}{2K_{L_1} + 1}. \quad (30)$$

In case of strong elastic deformation, after band crossover, practically all electrons are localized in Δ_1 -valleys ($n_{L_1} \approx 0$, $n_{\Delta_1} = 1/6$) and formula (30) are valid with change index $L_1 \rightarrow \Delta_1$.

The numeric results

In order to carry out the calculations it is necessary to know some parameters of the crystal, as well as of L_1 and Δ_1 valleys. All the parameters used to describe intravalley scattering in L_1 minima are well known [4–6]. The parameters necessary to describe the intervalley scattering have been mentioned in [1–3, 8, 9]. Different values of the effective masses and deformation potentials constants for Δ_1 valleys were estimated in [1–3, 9, 13, 14]. Unfortunately we haven't experimental data for the thermoEMF in case of strong hydrostatic pressure. For this reason we use the values of the effective masses and deformation potentials constants from [9] because this values give qualitative fit with experimental data for piezoresistance under strong hydrostatic pressure. Thus we use the values for effective masses in Δ_1 valleys $m_{\perp}^{\Delta_1}/m_0 = 0.225$, $m_{\parallel}^{\Delta_1}/m_0 = 0.612$ and for deformation potentials constants $C_1^{\Delta_1} = 0.1$ eV, $C_2^{\Delta_1} = 12.0$ eV. We use the value $C_1^{\Delta_1} = 0.18$ V and $C_2^{\Delta_1} = 8.636$ eV too, because this value describes quantitatively crossover between L_1 and Δ_1 valleys. In all figures below the continuous curves correspond first pair of constants and dotted curves correspond second pair of constants. We use values of elastic constants derived in [17]. Let us bring the results of the numerical calculations of diffusion thermoEMF and phonon drag thermoEMF using these parameters and other constants from [5, 6, 18]. The figures below show the results for deformation potentials, occupation numbers, diffusion thermoEMF and phonon drag thermoEMF at two temperatures $T = 78$ K and $T = 300$ K. The electron concentration is $N_0' = 4.7 \cdot 10^{13} \text{ cm}^{-3}$.

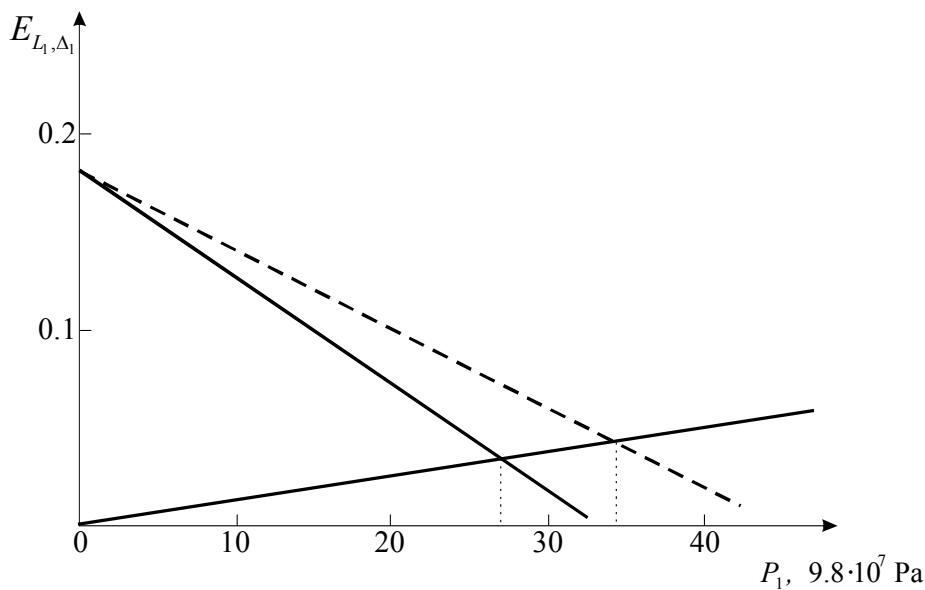


Fig. 1. Deformation potentials as function of P . $T=300\text{K}$.

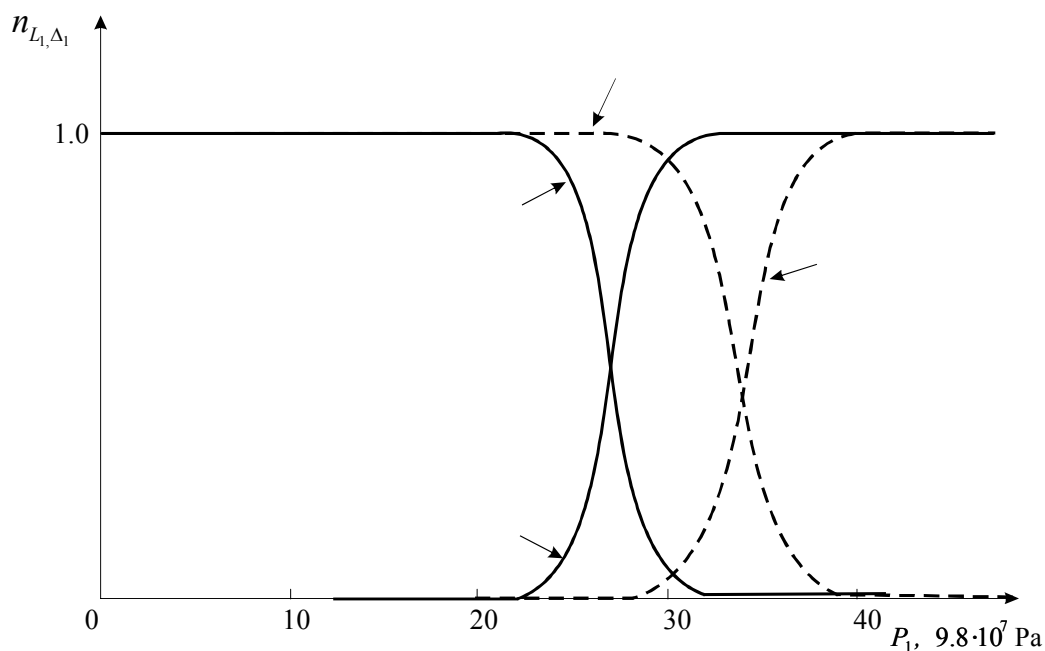


Fig. 2. Occupation numbers for L_1 - and Δ_1 -valleys as function of P . $T=78\text{ K}$.

Deformation potentials have temperature dependence only through elastic compliance tensor's component. This dependence is weak and on Fig. 1 respected dependences are demonstrated only for $T = 300\text{ K}$. The pressure P'_0 corresponds to the band crossover experimentally observed [3].

The result of the numeric calculations of diffusion thermoEMF as a function of applied hydrostatic pressure are shown on Fig. 4, 5. The value of diffusion thermoEMF in an undeformed crystal at given temperatures and electron concentration are equal to $\alpha^e(0; 78\text{ K}) = 1074\ \mu\text{V/K}$ and $\alpha^e(0; 300\text{ K}) = 1234\ \mu\text{V/K}$ respectively. The existence of the maximum (Fig. 3, 4) is explained in [8] for uniaxial pressure and in this case is similar too.

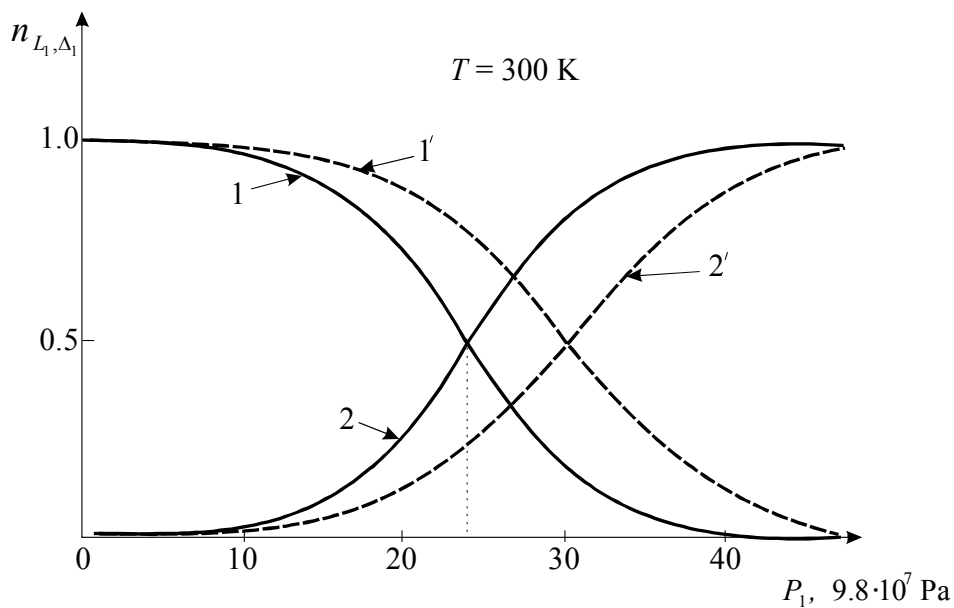


Fig. 3. Occupation numbers for L_1 - and Δ_1 - valleys as function of P . $T = 300 \text{ K}$.

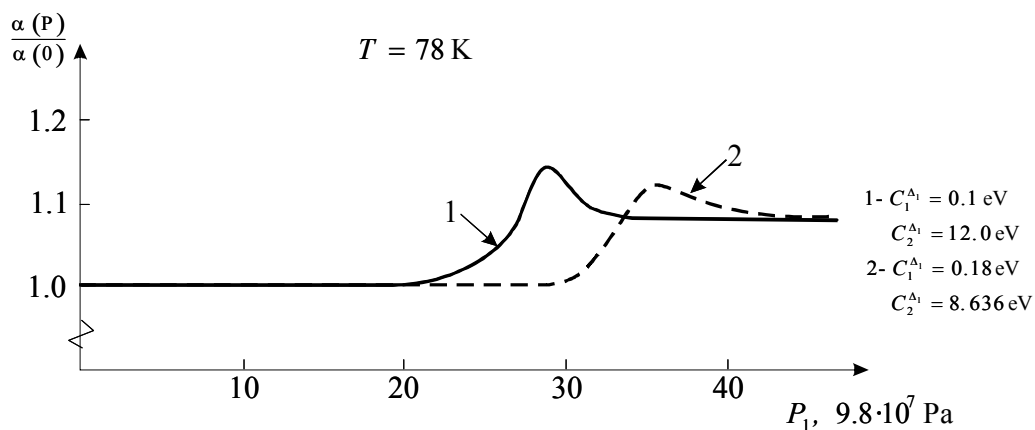


Fig. 4.

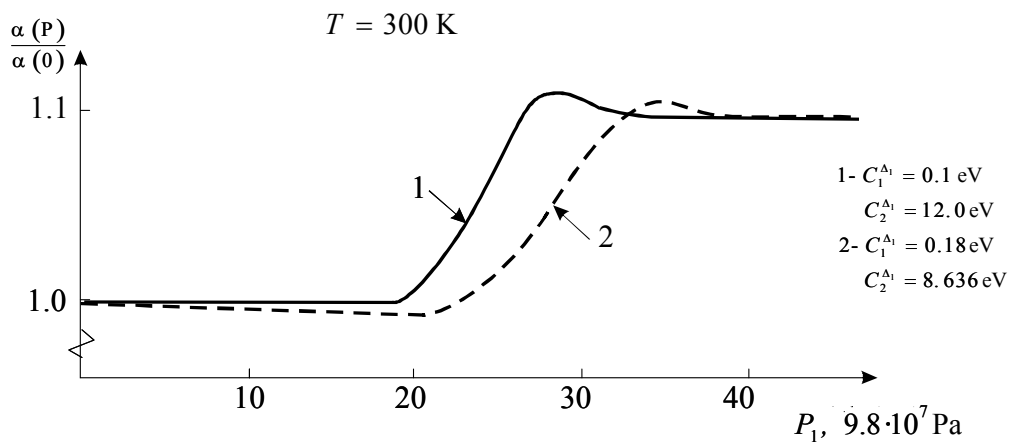


Fig. 5.

Variation of diffusion thermoEMF with hydrostatic pressure P ,
 $T = 78 \text{ K}$ (Fig. 4), $T = 300 \text{ K}$ (Fig. 5).

All parameters needful to calculate phonon drag thermoEMF have chosen as in [8]. Fig. 6, 7 show the results of the numerical calculation of the phonon drag thermoEMF in $L_1 - \Delta_1$ model of germanium under strong hydrostatic pressure. The shape of the curves is similar to the piezoresistance behaviour of the model [1–3]. It is obvious that in the region of high temperatures ($T = 300$ K) transition of the electrons between L_1 - and $\Delta_1^{(1,2)}$ - valleys begins at smaller values of P and, therefore, the interval of transition between L_1 - and $\Delta_1^{(1,2)}$ - valleys become even more “blurred”.

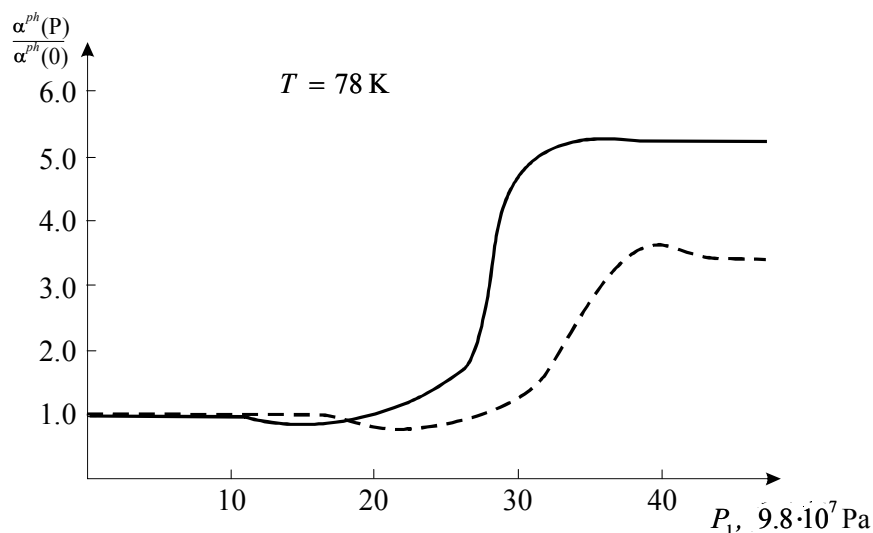


Fig. 6.

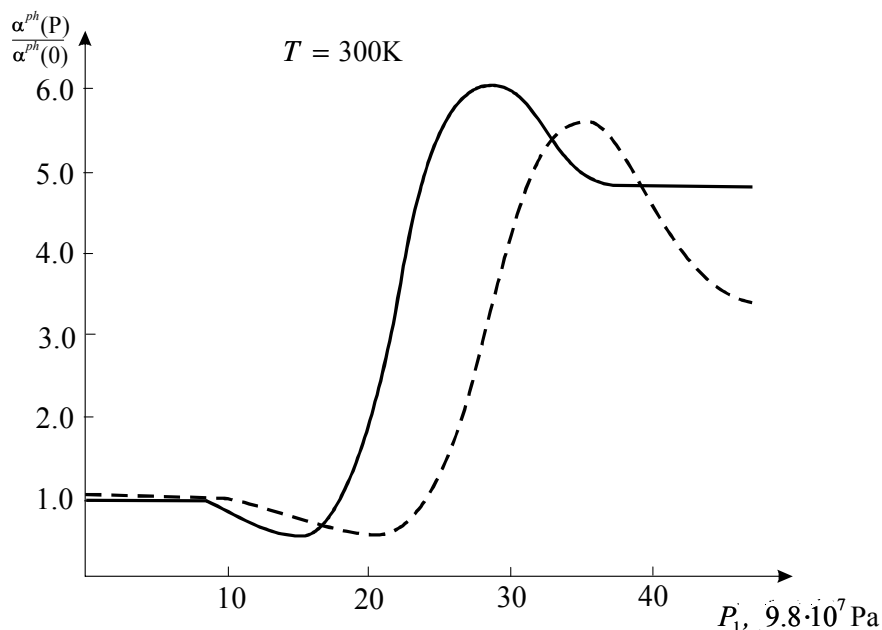


Fig. 7.

Variation of phonon drag thermoEMF with pressure P . $T = 78$ K (Fig. 6), $T = 300$ K (Fig. 7).

$$\alpha^{ph}(0; 78K) \approx 1000 \mu V/K, \quad \alpha^{ph}(0; 300K) \approx 6.0 \mu V/K.$$

The continuous curve corresponds $C_1^{\Delta_1} = 0.1$ eV, $C_2^{\Delta_1} = 12.0$ eV; the dotted curve corresponds

$$C_1^{\Delta_1} = 0.18$$
 eV and $C_2^{\Delta_1} = 8.636$ eV.

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