ISSN 2347-3487

Deformation potentials for Δ_1 minimum of conduction band of single crystals n-Ge

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ABSTRACT

Deformation potentials $\Xi_d^{\Delta} = -1{,}29\ eV$ and $\Xi_u^{\Delta} = 11{,}82\ eV$ for Δ_1 minimum of conduction band of single crystals *n-Ge* are defined on the basis of theory of the anisotropic scattering and experimental data of longitudinal piezoresistance for single crystals *n-Ge* for the case, when *P||J||[100]*. Pressure coefficients for Δ_1 minimum under uniaxial pressure along crystallographic directions *[100]*, *[110]*, *[111]* and hydrostatic pressure have been calculated taking into account the given parameters. The results show that the inversion of (L_1-Δ_1) type of absolute minimum in single crystals *n-Ge* can be implemented under hydrostatic and uniaxial pressures *P||J||[100]* and *P||J||[110]*.

Keywords: Uniaxial deformation, Pressure coefficient, Constants of deformation potential.

Council for Innovative Research

Peer Review Research Publishing System

Journal: Journal of Advances in Physics

Vol 5, No.1

japeditor@gmail.com

www.cirjap.com

ISSN 2347-3487

INTRODUCTION

Development of modern micro- and Nan electronics is determined to a large extent by the achievements of physics of semiconductors. Such semiconducting material as germanium has always been and remains one of the leading materials of modern semiconducting technology. It is used for the manufacture of diodes, triodes, power rectifiers, radiac instruments that measure the intensity of constant and variable magnetic fields [1], detectors for recording the particles of dark matter [2]. Also a single crystal germanium of n-type conduction is the main material as an optical environment for lenses, objectives, filters, which are used for area of 3-5 μm and 8-14 μm spectrum [3].

Single crystals of germanium with a minimum content of defects and impurities is a promising material for the needs of Nan electronics. Germanium which has no dislocation provides solutions to problems which arise in connection with the use of silicon in the process of nanoscaled transistor structures creation. The use of technologies for creation of uniaxial strain channels NMOSFET of electronic devices during replacing crystals *n-Ge* instead of *n-Si* allows to increase both the coefficient of amplification [4, 5] and the tunnel current [6]. The use of nanostructures with the self-induced *Ge/Si* Nan islands starts the new prospects for the development of opto- and Nan electronics [7]. Arrays of *Ge (GeSi)* quantum dots can be used successfully for the production of photo detectors for near infrared range and light emitted diodes for the same spectral region [8]. Nanostructures *Si/Ge* are the example of the strained germanium application [9]. In such nanostructures internal tensions which arise on the border of heterojunction due to the discrepancy of stable lattice of germanium and silicon, can additionally transform band structure and electronic spectrum. Results of the research in work [10] show that use of the uniaxial strain of 1.8% of germanium Nan wires tension reduces their resistivity in 30 times. Study of influence of the internal and external strain fields on the properties of such nanostructures and creation of different elements of functional electronics on their basis are the major problems in the management of their necessary electrical, optical, photoelectric, magnetic characteristics.

Shift of the semiconductor energy levels under the action of deformation and change of power spectrum of charge carriers which is connected with this process are the physical causes of deformation effects [11]. Constants of deformation potential are one of the most important quantitative parameters which determine rearrangement of the band structure of semiconductor under the action of deformation. All methods which are used for experimental determination of constants of the deformation potential, are usually based on researches related to the deformation of crystal. Uniaxial or comprehensive information is being used at such experiments. The value of constants of the deformation potential which have been obtained experimentally are used as well for the calculation of the energy shifts of appropriate semiconductor extremes as at different kind of deformation, and for calculation the probabilities of transition while scattering on the acoustic vibrations of lattice [12, 13]. As a rule, the use of a particular experimental method of determination the constants of deformation potential Ξ_u, and Ξ_d in single crystals of germanium allows to find the combination of the given constants [14-17]. Finding the values of constants of deformation potential Ξ_u та Ξ_d is a non-trivial task, which requires several experiments under different conditions for its solution. The authors of works [6,18] managed to define constants of deformation potential Ξ_u та Ξ_d for L_1 minimum. The author of work [19] performed theoretical calculations taking into account the constant of deformation potential Ξ_u which had been previously found in work18]. The results of work [19] show that the uniaxial deformation *n-Ge* has an effect as well on the value of the coefficient of absorption of light by free charge carriers, as on its dependence on the polarization of light. High energy minima of conduction band of the symmetry of Γ_2, Δ_1 and Γ_{15} can participate in the extreme conditions of directed significant electrical, strain, optical and thermal fields in a variety of kinetic and optical effects in *n-Ge* side by side with lowest (according to school of energy) L_1 minima. Parameters of the given minima are little known at present because considerable hydrostatic or uniaxial pressure are necessary for their determination. It is primarily a rather complex experimental task. There are only rare works about values of the effective mass, constants of deformation potential for given minima [20-22]. All these works have one trait in common. It lies in the fact that their final result is obtained on the basis of the data usage of unrelated studies of other authors. And it may make additional errors in the values of the required parameters. We managed to find the effective mass of density of states, tensor components of the effective mass and a combination of constants of deformation potential for Δ_1 minimum conduction band of crystals *n-Ge* in work [23] using only the experimental data of the longitudinal piezo resistance of crystals *n-Ge* and theory of anisotropic scattering.

Effective mass of charge carriers and expansion potential are tensors in the anisotropic semiconductors. Therefore, it is necessary to have tensors components of effective mass and constants of deformation potential in order to calculate various kinetic coefficients in such anisotropic semiconductors like germanium, silicon, gallium arsenide, cadmium antimonìd and other.

EXPERIMENTAL RESULTS

Therefore, in this work we've made a measurement of the longitudinal piezo resistance of single crystals *n-Ge* which had been alloyed by the impurity Sb with concentration $n=N_d=5\cdot10^{14}$ cm^{-3} under the temperature of liquid nitrogen in conditions when *P||J||[100]* (see Figure 1) in order to find constants of deformation potential Ξ_u and Ξ_d for Δ_1 minimum. Piezoresistance *n-Ge* under uniaxial pressures *P > 1,8 GPa* along crystallographic direction *[100]* (see Figure 1) is explained by deforming redistribution of electrons between four L_1 minima which ascend and two Δ_1 minima which descend at a scale of energies [20]. Presence of saturation of the piezo resistance n-Ge under uniaxial pressures *P > 2,4 GPa* (see Figure 1) indicates the implementation of (L_1-Δ_1) type inversion of an absolute minimum in crystals of

germanium. As for the entire range of uniaxial pressures (*0 < P < 2,6 GPa*) concentration of conduction by electrons $n=N_d=const$, then the mobility of electrons for Δ_1 minimum will be equal to:

$$\mu_{\Delta_1} = \frac{\rho_0}{\rho_\infty}\mu_{L_1}, \quad (1)$$

where $\frac{\rho_\infty}{\rho_0} = 7{,}05$ - quantity of piezo resistance *n-Ge* under uniaxial pressures *P > 2,4 GPa*, $\mu_{L_1} = 30100\ \frac{cm^2}{V\cdot s}$ - mobility of electrons for L_1 minimum (unstrained crystal).

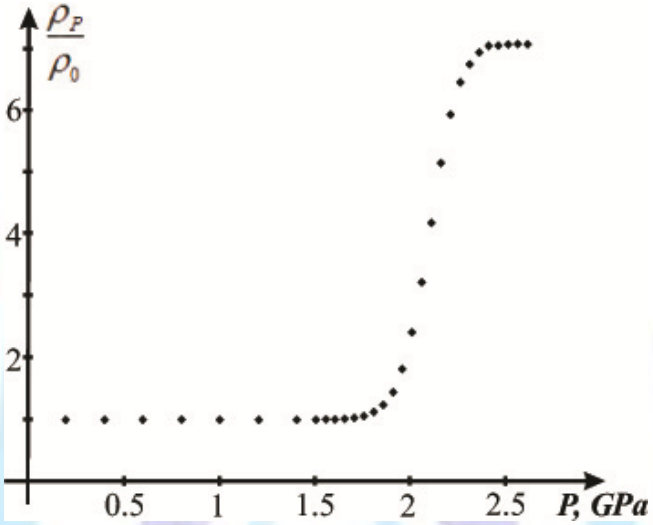

Fig 1: Piezoresistance of the uniaxially deformed along the crystallographic direction *[100]* single crystals *n-Ge* under T=77 K.

Then, in accordance with (1), $\mu_{\Delta_1} = 4270\ \frac{cm^2}{V\cdot s}$.

THE RESULTS OF THEORETICAL CALCULATIONS

Constant energy surfaces for both L_1 and Δ_1 minima are ellipsoids of rotation. Mobility of charge carriers in an unrestricted direction can be determined from the ratio [24]:

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

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 (2), for the Δ_1 minimum, when *P||J||[100]*

$$\mu_{\Delta_1} = \mu_\parallel . \quad (3)$$

On the other hand mobility tensor components can be expressed in tensor components of relaxation times and effective masses for the corresponding minimums:

$$\mu_\parallel = \frac{e}{m_\parallel} < \tau_\parallel > . \quad (4)$$

On the basis of the theory of anisotropic scattering an expression for the longitudinal tensor component of relaxation times $\tau_\parallel$ under conditions of mixed scattering of electrons by acoustic phonons and impurity ions will be as following [25]:

$$\tau_\parallel = \frac{a_\parallel}{\sqrt{k_Б}T^{\frac{3}{2}}} \cdot \frac{x^{\frac{3}{2}}}{x^2 + b_0}, \quad (5)$$

$$a_{\parallel} = \frac{\pi C_{11}\hbar^4}{k\Xi_d^2\sqrt{2m_{\parallel}m_{\perp}^2}}\cdot\frac{1}{\Phi_{0a}}, \qquad b_0 = \frac{a_{\parallel}\cdot\Phi_{0i}}{\sqrt{k}T^{\frac{3}{2}}\tau_{0i}(kT)}, \tag{6}$$

$$\tau_{0i}(kT) = \frac{\sqrt{2}m_{\perp}\varepsilon^2(kT)^{\frac{3}{2}}}{\pi Ne^4\sqrt{m_{\parallel}}}, \tag{7}$$

$$\Phi_{0a} = 1+\frac{2(1+\beta^2)}{\beta^2}\left(1-\frac{3}{\beta^2}+\frac{3}{\beta^3}\alpha\right)\frac{\Xi_u}{\Xi_d}+ \\ +\frac{(1+\beta^2)}{\beta^4}\frac{\Xi_u^2}{\Xi_d^2}\left((1+\beta^2)\left(1-\frac{6}{\beta^2}-\frac{3}{2\beta^2(1+\beta^2)}+\frac{15\alpha}{2\beta^3}\right)+\frac{C_{11}}{C_{44}}\left(2+\frac{15}{2\beta^2}-\frac{3}{2\beta^3}(5+3\beta^2)\alpha\right)\right) \tag{8}$$

$$\Phi_{0i} = \frac{3}{2\beta^3}\left(\left(\frac{\beta}{1+\beta^2}-\alpha\right)\ln\gamma^2-\alpha\ln(1+\beta^2)+2L(a)+\frac{\beta\gamma^2}{2}\left(\frac{\beta^2-1}{\beta^2+1}+\frac{\alpha(\beta^2+1)}{\beta}\right)\right), \tag{9},$$

where $\alpha = arctg\ \beta$, $\beta^2 = \frac{m_{\parallel}-m_{\perp}}{m_{\perp}}$, $\gamma = \sqrt{\frac{\pi\hbar^2e^2N}{2m_{\parallel}\varepsilon kT}}$, $L(a) = -\int_0^{\alpha}\ln\cos\varphi d\varphi$ – Lobachevskyi function,

N - concentration of impurity.

For degenerate electron gas

$$\left\langle\tau_{\parallel}\right\rangle = \frac{4}{3\sqrt{\pi}}\int_0^{\infty}dx x^{\frac{3}{2}}e^{-x}\tau_{\parallel}\ . \tag{10}$$

As it follows from the expressions (3-10), mobility of electrons for Δ_1 minimum is dependent on the elastic constants C_{11} and C_{44}, tensor components of the effective mass $m_{\parallel}$ and $m_{\perp}$, deformation potential Ξ_u and Ξ_d. Elastic steels $C_{11} = 1{,}292\cdot10^{11}$ Pa and $C_{44} = 0{,}67\cdot10^{11}$ Pa for single crystals of germanium are the well-known parameters [26]. Effective masses $m_{\parallel} = 1{,}65m_0$ and $m_{\perp} = 0{,}32m_0$ for Δ_1 minimum have been found by us in found by us in the work [23]. Combination of constants of deformation potential:

$$0{,}35\Xi_d + 0{,}77\Xi_u = 8{,}65\,\text{eV} \tag{11}$$

has also been obtained by us in the work [23].

According to expressions (3-11), we obtain a system of equations for finding constants of deformation potential Ξ_u and Ξ_d:

$$\begin{cases}\dfrac{4ea_{\parallel}}{3\sqrt{\pi k_Б}m_{\parallel}T^{3/2}}\displaystyle\int_0^{\infty}\frac{x^3e^{-x}dx}{x^2+b_0} = \mu_{\Delta_1},\\ 0{,}35\Xi_d + 0{,}77\Xi_u = 8{,}65.\end{cases} \tag{12}$$

Solution of system of equations (12) gives the following value of constants of deformation potential for Δ_1 minimum: $\Xi_u = 11{,}82$ eV **та** $\Xi_d = -1{,}29$ **eV.**

It is necessary to have also values of baric coefficients for different types of conduction band minima in order to explain various kinetic and optical effects in the strongly deformed crystals n-Ge side by side with such important parameters of band structure, as the constants of deformation potential, components of the tensor effective masses.

Therefore, we'll calculate baric coefficients for Δ_1 minimum and change of magnitude of the energy gap between L_1 and Δ_1 minima of crystals *n-Ge* conduction band under hydrostatic and uniaxial pressures. Data of work [27] point out to the fact that shift in according with the scale of energies under elastic deformation of L_1 four minima and Δ_1 six minima is equal correspondingly:

$$\begin{cases} \Delta E_1 = \left(\Xi_d + \frac{1}{3}\Xi_u\right)\left(\varepsilon_{11}+\varepsilon_{22}+\varepsilon_{33}\right)+\frac{2}{3}\left(\varepsilon_{12}+\varepsilon_{13}+\varepsilon_{23}\right), \\ \Delta E_2 = \left(\Xi_d + \frac{1}{3}\Xi_u\right)\left(\varepsilon_{11}+\varepsilon_{22}+\varepsilon_{33}\right)+\frac{2}{3}\left(\varepsilon_{23}-\varepsilon_{12}-\varepsilon_{13}\right), \\ \Delta E_3 = \left(\Xi_d + \frac{1}{3}\Xi_u\right)\left(\varepsilon_{11}+\varepsilon_{22}+\varepsilon_{33}\right)+\frac{2}{3}\left(\varepsilon_{13}-\varepsilon_{12}-\varepsilon_{23}\right), \\ \Delta E_4 = \left(\Xi_d + \frac{1}{3}\Xi_u\right)\left(\varepsilon_{11}+\varepsilon_{22}+\varepsilon_{33}\right)+\frac{2}{3}\left(\varepsilon_{12}-\varepsilon_{13}-\varepsilon_{23}\right). \end{cases}, \quad (13)$$

and

$$\begin{cases} \Delta E_{1,2} = \Xi_d\left(\varepsilon_{11}+\varepsilon_{22}+\varepsilon_{33}\right)+\Xi_u\varepsilon_{11}, \\ \Delta E_{3,4} = \Xi_d\left(\varepsilon_{11}+\varepsilon_{22}+\varepsilon_{33}\right)+\Xi_u\varepsilon_{22}, \\ \Delta E_{5,6} = \Xi_d\left(\varepsilon_{11}+\varepsilon_{22}+\varepsilon_{33}\right)+\Xi_u\varepsilon_{33}, \end{cases} \quad (14)$$

where ε_{ij} – deformation tensor components.

For hydrostatic pressure *P*

$$\varepsilon_{ij} = -\frac{P}{3K}\delta_{ij}, \quad (15)$$

where $K = \frac{1}{3}\left(C_{11}+2C_{12}\right)$ – module of comprehensive pressure, δ_{ij} – Kronecker symbol.

For the case of uniaxial pressures along the crystallographic directions *[100], [110]* and *[111]* expressions for deformation tensor components are equal:

$$\begin{cases} \varepsilon_{ii} = -P\dfrac{\left(C_{11}+2C_{12}\right)n_i^2 - C_{12}}{\left(C_{11}-C_{12}\right)\left(C_{11}+2C_{12}\right)}, \\ \varepsilon_{ij} = -P\dfrac{n_i n_j}{2C_{44}}, i \neq j, \end{cases} \quad (16)$$

where n_i and n_j – components of the unit vector of normal, which is directed along the direction of the uniaxial pressure, is linked with crystallographic axes in the coordinate system *[100], [110]* та *[111]*.

Taking into consideration values of elastic constants $C_{11} = 1{,}292 \cdot 10^{11}\ Pa$, $C_{12} = 0{,}479 \cdot 10^{11}\ Pa$, $C_{44} = 0{,}67 \cdot 10^{11}\ Pa$ [26], constants of deformation potential $\Xi_u = 16{,}4\ eV$ and $\Xi_d = -6{,}4\ eV$ for L_1 minimum [18] and corresponding constants $\Xi_u = 11{,}82\ eV$ and $\Xi_d = -1{,}29\ eV$ for Δ_1 minimum (which have been found by us), it is possible to find on the basis of expressions (13-16) baric coefficients for Δ_1 minimum and change of magnitude of the energy gap between L_1 and Δ_1 minima of conduction band of single crystals *n-Ge* under hydrostatic and uniaxial pressure. Results of the given calculations are presented in the Table 1.

Table 1. Values of baric coefficients for Δ_1 minimum and change of magnitude of the energy gap between L_1 and Δ_1 minima of single crystals *n-Ge* conduction band.

Pressure	Pressure coefficients for Δ_1 minimum $\frac{dE_{\Delta_1}}{dP}\cdot 10^{11}, \frac{eV}{Pa}$	Change of magnitude of the energy gap between L_1 and Δ_1 minima $\frac{dE_{(L_1-\Delta_1)}}{dP}\cdot 10^{11}, \frac{eV}{Pa}$
Uniaxial pressure *P||[100]*	-8,65	-8,97
Uniaxial pressure *P||[110]*	-5,9	-2,24
Uniaxial pressure *P||[111]*	-0,92	6,73
Hydrostatic pressure	-2,77	-3,75

In work [28] on the basis of measurements of tensity resistive effect under hydrostatic pressure baric coefficient for Δ_1 minimum $\frac{dE_{\Delta_1}}{dP} = -(2{,}4 \pm 0{,}4)\cdot 10^{11}\frac{eV}{Pa}$ have been found, which accords well to within the limits of error with its correspondent value that have been calculated by us. According to the data of Table 1, an energy gap between L_1 and Δ_1 minima of single crystals n-Ge conduction band decreases under hydrostatic and uniaxial pressures along the crystallographic directions *[100]* and *[110]* which allows to realize inversion of type (L_1 - Δ_1) absolute minimum.

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