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Electron and hole effective masses in heavily boron doped silicon nanostructures determined using cyclotron resonance experiments

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Abstract. We present the experimental and theoretical results of analysis of the optically-induced cyclotron resonance measurements carried out using the charge carriers in silicon (Si) nanostructures at 9 GHz and 4 K. Effective mass values for electrons were determined as $m_{el}^* = 0.93m_0$ and $m_{el}^* = 0.214m_0$. The obtained value of the transversal mass is higher than that reported for bulk Si. Parameters defining the energy surfaces near the valence band edge for heavy and light holes were found to be equal: $A = -4.002$, $B = 1.0$, $C = 4.025$, and corresponding to the experimental effective masses obtained in three orientations of the magnetic field: $m_{lh}^{*[001]} = 0.172$, $m_{lh}^{*[111]} = 0.157$, $m_{lh}^{*[110]} = 0.163$, and $m_{hh}^{*[001]} = 0.46$, $m_{hh}^{*[111]} = 0.56$, $m_{hh}^{*[110]} = 0.53$. The obtained energy band parameters and effective masses for holes have coincided with those found in bulk Si. The average values of the relaxation time of the charge carriers are found to be: $\tau_{e,1} = 2.28\cdot10^{-10}$ s; $\tau_{e,2} = 3.57\cdot10^{-10}$ s; $\tau_{lh} = 6.9\cdot10^{-10}$ s; $\tau_{hh} = 7.2\cdot10^{-10}$ s, which are by one order of value larger than those obtained in bulk Si. The prolongation of the transport time for photo-excited electrons and holes can be explained by the spatial separation of electrons and holes in the field of the p^+-n junction as well as by reduction of the scattering process due to the presence of boron dipole centers.
Keywords: cyclotron resonance, effective mass, relaxation time, silicon nanostructure.

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1. Introduction

In recent years, one of the directions in the development of semiconductor nanoelectronics is production and investigation of self-ordered quantum wells, wires, and dots with the aim of fabricating single-electron transistors and memory cells demonstrating the effects of individual carrier transport up to room temperature [1, 2]. The variety of these nanostructures can find application in spintronic devices that are based on spatial variation in their spin projections [3] instead of on the transport of electrons and holes. In particular, a special attention is given to the so-called hybrid systems or nanosandwiches representing silicon (Si) nanostructures in the negative-U shells [3]. The basis of one such nanosandwich is an ultra-narrow *p*-type Si quantum well (SQW) confined by heavily boron doped δ-shaped barriers on the *n*-type Si (100) surface shown in Figs. 1a and 1b. The observed progress in the development of these Si nanostructures has stimulated interest to their electronic and structural properties, in particular, to understand how their energy band structure is fitting with that of bulk Si material. It is well known that an informative method to probe the energy band structure both in bulk semiconductors and in nanostructures is the cyclotron resonance (CR) technique.

It was previously shown that optically induced CR could be observed in Si nanosandwiches. The

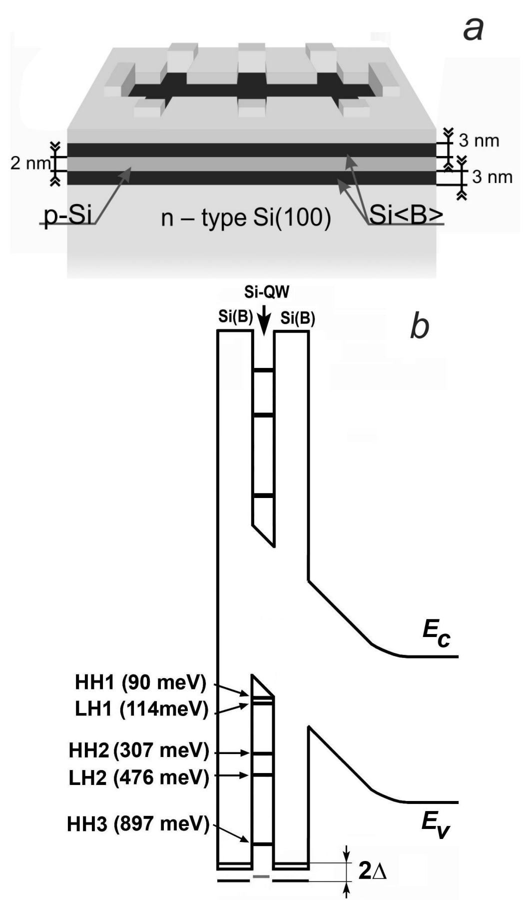

Fig. 1. Experimental structure of the Si nanosandwich prepared within the Hall geometry on the basis of an ultra-narrow *p*-type SQW confined by δ-shaped barriers heavily doped with boron on an *n*-type Si (100) surface (Reproduced from [3]). The vertical gate is intended for controlling the 2D hole density and the intensity of spin-orbit interaction in QW.

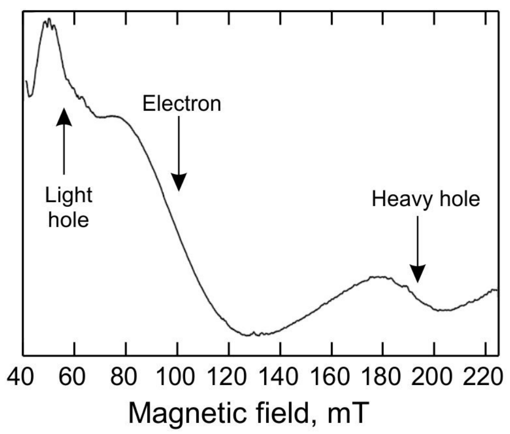

Fig. 2. Typical X-band CR spectrum for SQW p^+-n junction on {100}-Si, magnetic field $\vec{H}$ within the {110} plane perpendicular to the {100}-interface ($\vec{H} \parallel \langle 100\rangle - 20°$) under illumination with light of the wavelength 577 nm. $T = 4$ K.

investigations of CR in Si nanosandwiches were carried out at 3.8 K using the X-band electron spin resonance (ESR) technique. It was shown that despite an ultrahigh boron concentration of $5{\cdot}10^{21}$ cm^{-3} in the δ-shaped barriers, the Si nanosandwiches are characterized by a large momentum relaxation time (transport time) $\tau_m > 5{\cdot}10^{-10}$ s for heavy and light holes, which is sufficiently long to observe the CR, $\omega_c\tau_m \geq 1$ [4]. Besides, two sets of parameters that define the energy surfaces near the valence band edge were found for heavy and light holes. The obtained values are close to those found for holes in bulk Si. At the same time, a significant discrepancy between parameters obtained for holes in bulk Si single crystal and heavy holes in Si nanosandwiches (A = –4.15, $|B|$ = 2.75, $|C|$ = 1.70) has been found using the optically detected CR technique by measuring the impurity photoluminescence enhancement [5].

This fact indicates that the effective mass values depend on the used CR experimental technique that is able to select the contribution from the free electrons and holes as well as carriers at quantum-dimensional subbands of the Si nanosandwich [3-5].

To this end in this work, we provide careful control of the effective mass values for electrons and holes by means of a classical CR to determine the influence of the Fermi level position on the anisotropy of the electron/hole effective mass in quantum-dimensional Si structures.

2. Experimental results

Self-assembled Si quantum-wells (SQW) that are separated by the δ-barrier heavily doped with boron was studied by ESR at X-band frequencies under low temperatures. Cyclotron resonance (CR) from the electrons, light and heavy holes was observed in low magnetic fields at $T = 4$ K under band gap illumination. Fig. 2 shows optically induced CR spectrum registered in heavily doped SQW p^+-n junctions.

Fig. 3 shows the angular dependence of the CR spectrum observed for an SQW p^+-n junction on {100}-Si. The optimal wavelength light for CR observation was

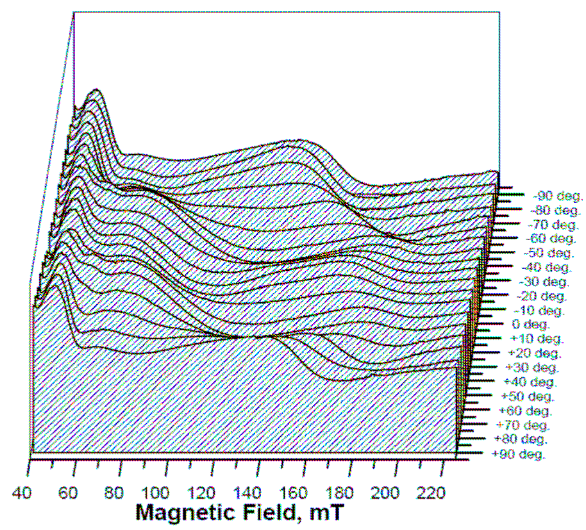

Fig. 3. The angular dependence of CR spectra for SQW p^+-n junction on {100}-Si. Rotation of the magnetic field $\vec{H}$ in a {100}-plane perpendicular to a {100}-interface (0° = $\vec{H}$ ∥ interface, ±90° = $\vec{H}$ ⊥ interface). $T = 4$ K, ω = 9.45 GHz, λ = 577 nm.

Table 1. The resonance fields H_{0i} and widths ΔH_i of the CR line obtained by fitting Eq. (1) with experimental spectra. θ is the angle between $\vec{H}$ and [001] direction.

H_{0i}, ΔH_{0i} (mT)	θ, deg.										
	90	80	70	60	54	50	40	30	20	10	0
H_{0e1}	149	142	129	112	99	100	90	83	77	73	72
H_{0e2}	89	89	93	96	99	96	106	116	126	142	145
H_{0lh}	55	54	54	54	53	53	54	55	56	58	59
H_{0hh}	179	179	182	182	190	189	179	175	165	155	149
ΔH_{e1}	50	50	50	48	45	45	40	40	35	35	35
ΔH_{e2}	35	35	35	30	35	40	40	40	50	50	50
ΔH_{lh}	9	9	9	9	8	8	9	9	9	9	10
ΔH_{hh}	30	30	35	35	30	28	25	25	20	30	30

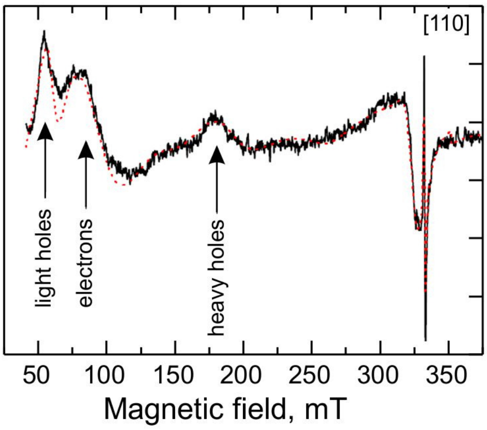

Fig. 4. The CR spectrum recorded at $\vec{H}$ ∥ [110]. The dashed line is a fit with Eq. (1). Arrows stand for the peaks due to the light and heavy holes as well as electrons from the energy valleys with the long axis parallel and perpendicular to the magnetic field $\vec{H}$ direction, respectively.

found to be 577 nm. The external magnetic field $\vec{H}$ was rotated within the {100}-plane perpendicular to a {100}-interface (0° = $\vec{H}$ ∥ interface, ±90° = $\vec{H} \perp$ interface).

As can be seen from Fig. 3, the shift of CR line due to the heavy holes was observed for the rotation of the magnetic field in the {100} plane, which was caused by the effect of the confining potential that is able to create the built-in electrical field inside ultra-shallow boron diffusion profile and its different arrangement in longitudinal and lateral SQW. This electrical field may also enhance the optically-detected CR.

3. Theory of CR of electrons and holes in SQW

The frequency of the resonance peak can be used as a mean to determine the effective masses of electrons and holes, since the frequency ω and the magnetic field $\vec{H}$ can be measured, and m^* is unknown. Taking into account Eq. (8) from [6] and Eq. (15) from [7], one can obtain the CR lineshape in the presence of the modulation field (*i.e.*, the recorded derivative of the absorption curve d*P*/d*H*) in terms of magnetic field:

$$f(H) = \sum_i I_i \left(\frac{\left(1+\left(H^2-H_{0i}^2\right)/\Delta H_i^2\right)^2}{4\left(H_{0i}/\Delta H_i\right)^2+\left(1+\left(H^2-H_{0i}^2\right)/\Delta H_i^2\right)^2} + \right.$$
$$\left. + \frac{4\left(H_{0i}^2-H^2\right)/\Delta H_i^2 - 2 + 2\left(H_{0i}^4-H^4\right)/\Delta H_i^4}{4\left(H_{0i}/\Delta H_i\right)^2+\left(1+\left(H^2-H_{0i}^2\right)/\Delta H_i^2\right)^2} \right), \quad (1)$$

where $\Delta H_i/H_{0i} = 1/\omega\tau_i$ is the CR linewidth for the i^{th} component, $H_{0i} = \omega \cdot m_i^* \cdot c/e$ – resonance magnetic field value, ω – microwave frequency, τ – relaxation time of the charge carriers (carrier free path time), m_i^* is cyclotron effective mass of the corresponding charge carriers, *e* – particle's charge.

Fitting the Eq. (1) with the experimental spectrum allows one to obtain the resonance fields H_{0i} and linewidth $\Delta H_i = m_i^* \cdot c \cdot \tau^{-1}/e$. The H_0 value and microwave frequency are related by the expression $H_{0i} = \left(m_i^*/m_0\right) m_0 \cdot c \cdot \omega/e = 3372.06\left(m_i^*/m_0\right)$, where m_0 is the free electron mass. The CR line resonance fields and widths obtained by fitting the Eq. (1) with the experimental spectra are given in Table 1.

Table 2. Cyclotron masses of electrons (m_{e1}^*, m_{e2}^*), light holes (m_{lh}^*) and heavy holes (m_{hh}^*), obtained from the analysis of the CR spectra observed in SQW. The magnetic field $\vec{H}$ rotates from [001] to $[1\bar{1}0]$. θ is the angle between $\vec{H}$ and [001] direction.

m_i^*/m_0	θ, deg.										
	90	80	70	60	54	50	40	30	20	10	0
m_{e1}^*/m_0	0.44	0.42	0.37	0.27	0.29	0.28	0.28	0.25	0.23	0.21	0.20
m_{e2}^*/m_0	0.26	0.26	0.26	0.27	0.29	0.28	0.31	0.34	0.37	0.42	0.44
m_{lh}^*/m_0	0.163	0.160	0.160	0.160	0.157	0.157	0.160	0.163	0.166	0.172	0.175
m_{hh}^*/m_0	0.53	0.53	0.54	0.54	0.56	0.55	0.53	0.52	0.49	0.46	0.44

Table 3. Cyclotron masses of electrons ($m^*_{e\|}$, $m^*_{e\perp}$) and holes (m^*_{hh}, m^*_{lh}) in Si nanostructure and in bulk Si found in [9-12] for three orientations of the magnetic field.

$m^*_{e\|}$	$m^*_{e\perp}$	$m^{*[001]}_{hh}$	$m^{*[001]}_{lh}$	$m^{*[111]}_{hh}$	$m^{*[111]}_{lh}$	$m^{*[110]}_{hh}$	$m^{*[110]}_{lh}$	Ref.
0.93	0.214	0.46	0.172	0.56	0.157	0.53	0.163	This work
0.96	0.16	0.26	0.18	0.67	0.13	0.54	0.14	[9]
0.92	0.19							[10]
0.98±0.04	0.19±0.01	0.46	0.17	0.56	0.16	0.53	0.16	[11]
		0.43	0.19	0.27		0.43	0.24	[12]

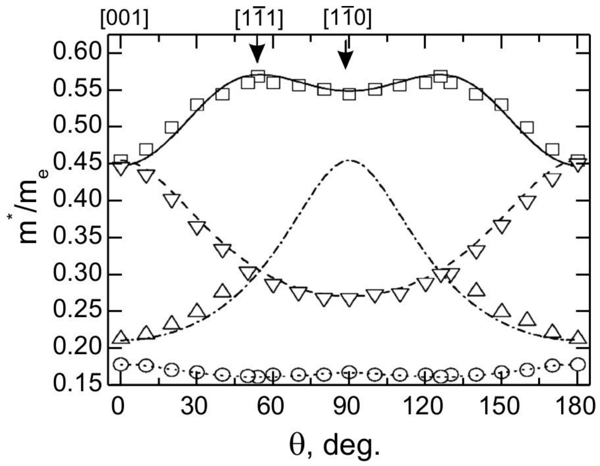

Fig. 5. The angular dependence of the effective masses for electrons m^*_{e1} (△), m^*_{e2} (▽), light holes m^*_{lh} (○), and heavy holes m^*_{hh} (□). Solid, dashed, dotted and dot-dashed curves are fits with Eq. (2) and Eq. (4) for electrons and holes, respectively.

Fig. 4 shows fitting the Eq. (1) with the experimental spectrum for the case when $\vec{H}\parallel[110]$.

As can be seen from Fig. 4, two CR lines due to the heavy and light holes and two CR signals due to electrons were resolved in CR spectrum for the $\vec{H}\parallel[110]$. Two CR signals from electrons belong to the different energy valleys with the ellipsoid long axis $\vec{c}\parallel\vec{H}$ and the other to the ellipsoid with $\vec{c}\perp\vec{H}$ in directions near $\vec{H}\parallel[110]$ or $\vec{H}\parallel[001]$, respectively. When $\vec{H}\parallel[1\bar{1}1]$, three valleys become equivalent, and only a single CR signal is observed near this direction. The m^*_i/m_0 values can be obtained from $m^*_i/m_0 = H_{0i}/3372$ and are adduced in Table 2 as a function of the crystal orientation.

According to Shokley [8], the cyclotron mass m^*_c corresponding to the resonance peak is related with the band effective mass tensor $m^*_{e\|}$, and $m^*_{e\perp}$ can be given for electrons by:

$$m^*_c = \left(m^*_{e\|}\cdot m^*_{e\perp}\Big/\left(m^*_{e\|}\cos^2\theta + m^*_{e\perp}\sin^2\theta\right)\right)^{1/2}, \qquad (2)$$

where θ is the angle between the magnetic field $\vec{H}$ and the elongated axis of ellipsoids that are oriented along [100], [010], [001] cubic axes.

Although the plane of the Si substrate is (001) plane, it is not the fact that the final orientations of the wells and barriers in the multilayer are the same as in the substrate. The effective masses of electrons and holes for [001], [111], [110] orientations of the magnetic field in Si nanostructure and in bulk Si taken from [9-12] are listed in Table 3.

From comparison of the effective masses of electrons in bulk Si listed in Table 3 for [001], [111], [110] orientations with those obtained in the Si nanostructure, it follows that the magnetic field in our experiment lies in the (110) plane.

The fact that two CR signals were observed for electrons at $\vec{H}\parallel[110]$ and they merge into one when the magnetic field is around [111] direction served as an evidence that the magnetic field is rotated in the (110) plane. Fig. 5 shows the angular dependence of the effective masses for electrons, light and heavy holes. In Fig. 5, the angle $\theta = 0$ corresponds to $\vec{H}\parallel[001]$, at which two CR signals from electrons are observed, but the CR signal from prolonged energy valley is more intensive. At $\vec{H}\parallel[111]$ single CR signal is observed, while at $\vec{H}\parallel[1\bar{1}0]$ CR signals from the two valleys oriented along [100] and [010] axes are observed. The dashed and point-dashed curves represent fits of the experimental angular dependences with Eq. (2), when using the fitting parameters of m^*_e: $m^*_{e\|} = 0.93m_0$ and $m^*_{e\perp} = 0.214m_0$. The obtained value of the transversal mass is larger than that reported for bulk Si (see Table 3).

If we compare the effective masses for heavy holes m^*_{hh}/m_0 given in Table 3, it is seen that they have close values in directions [001], [110], and [111]. However, the values of the effective masses for the light holes m^*_{lh}/m_0 are shifted with respect to those obtained for the light holes in bulk Si for three main orientations. In order to be sure that we observe CR from the SQW structure, and not from the Si substrate, it is necessary to calculate energy band parameters *A*, *B*, *C* with the maximum accuracy. The constant energy surface for holes in the bulk Si has the form [6, 12]:

$$E(k) = Ak^2 \pm \left[B^2k^4 + C^2\left(k_x^2k_y^2 + k_x^2k_z^2 + k_y^2k_z^2\right)\right]^{1/2}. \qquad (3)$$

The effective masses of holes were obtained in [6] for the case of $\vec{H}$ rotating in the (110) plane through the parameters *A*, *B*, *C* as

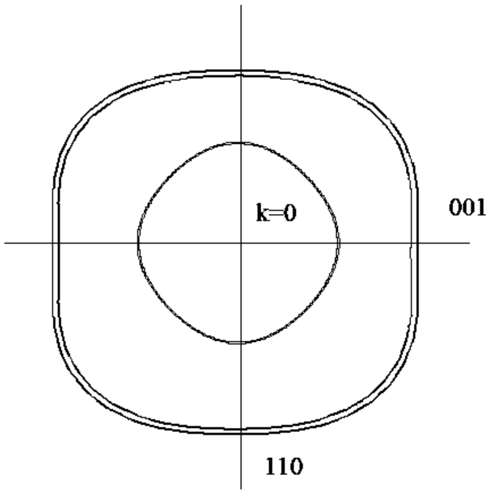

Fig. 6. The contours of the valence band constant energy surface in the (110) plane plotted for A, B, C parameters found in this work and taken from [12]. Outer contour for heavy hole corresponds to $A = -4.002$, $B = 1.0$, $C = 4.025$, the inner contour is plotted for $A = -4.0$, $B = 1.1$, $C = 4.1$. The contours for light holes for Si and SQW coincide.

$$m^*(\theta)/m_0 = \frac{2}{\pi}\int_0^{\pi/2} \frac{d\varphi}{A \pm \left[B^2 + 0.25C^2\left(1 + g(\theta,\varphi)\right)\right]^{1/2}} \quad (4)$$

with

$$g(\theta,\varphi) = -\left(3\cos^2\theta - 1\right)\left(\cos^4\varphi \cdot \left(\cos^2\theta - 3\right) + 2\cos^2\varphi\right).$$

Usually, to calculate $m^*(\theta)$, expansion of Eq. (4) in powers of $g(\varphi)$ is used.

We have made the precise integration of the Shokley integral (Eq. (4)) over the angle φ for the set of different values A, B, C and θ. At $\vec{H} \parallel [111]$, $g(\theta, \varphi) = 0$, Eq. (4) is simplified:

$$m^*\left(\theta = 54.7^\circ\right)/m_0 = 1\Big/\left[A \pm \left(B^2 + 0.25C^2\right)^{1/2}\right]. \quad (5)$$

Eq. (5) allows us to obtain at once the values $A = 4.002$ and $(B^2 + 0.25C^2) = 5.052$ from $m_0 \cdot \left(\left(m_{lh}^*\right)^{-1} + \left(m_{hh}^*\right)^{-1}\right)$ with m_{lh}^* and m_{hh}^* values taken from Table 2.

Integration of Eq. (4) at $\theta = 0$ with the known A and $(B^2 + 0.25C^2)$ and comparison with the experimental values m_{lh}^* and m_{hh}^* allows to find all the parameters $A = -4.002$, $B = 1.0$ and $C = 4.025$, corresponding to the experimental effective masses. Fig. 5 demonstrates the agreement between calculated values $m^*(\theta)$ using Eq. (4) and experimental values given in Table 2. The obtained values of A, B, C show that variation of the valence band structure near the top of the band is small in comparison with the bulk Si. In accordance with [12], in a bulk Si $A = -4.0$, $B = 1.1$, $C = 4.1$, which indicates that variations of the parameters are negligible.

It is possible to find the lifetime for electrons and holes from the equation $\Delta H_i/H_{0i} = 1/\omega\tau_i$, where $\omega = 0.925\cdot10^{10}\ \text{s}^{-1}$ is the microwave frequency, ΔH_i and H_{0i} are given in Table 1. The average values τ_i were found to be equal to $\tau_{e1} = 2.28\cdot10^{-10}$ s; $\tau_{e2} = 3.57\cdot10^{-10}$ s; $\tau_{lh} = 6.9\cdot10^{-10}$ s; $\tau_{hh} = 7.2\cdot10^{-10}$ s. The obtained lifetimes are by one order of value larger than those obtained in bulk Si in [6] ($\tau_{e1} = 7\cdot10^{-11}$ s; $\tau_{lh} = 7\cdot10^{-11}$ s; $\tau_{hh} = 6\cdot10^{-11}$ s). This fact confirms that we observed CR from band charge carrier.

Fig. 6 shows the contours of the valence band constant energy surface in the (110) plane in SQW and bulk Si. The contours of the valence band surface of the heavy holes for the SQW is noticeably extended in comparison with those of bulk Si, while the contours of the valence band surface of the light holes for SQW and bulk Si coincides.

4. Conclusions

Optically-induced CR at X-band frequency was used to study electron and hole effective masses in Si nanosandwich representing the ultra-narrow *p*-type SQW confined by the δ-shaped barriers heavily doped with boron on the *n*-type Si (100) surface. The CR angular dependences reveal the anisotropy of both the electron/hole effective mass in Si bulk and Landau levels scheme in the SQW. Fitting the experimental angular dependence of the CR signals from electrons with the usual cyclotron mass relation for the case of an ellipsoidal energy surface, the values of electron effective masses $m_{e\parallel}^* = 0.93m_0$ and $m_{e\perp}^* = 0.214m_0$ were obtained. The obtained value of the transversal mass is larger than that reported for bulk silicon. The parameters A, B, C that define the energy surfaces near the valence band edge for heavy and light holes have been evaluated by fitting the experimental and theoretical angular dependences of their effective masses. It was found that $A = -4.002$, $B = 1.0$, $C = 4.025$ fit well with the effective masses: $m_{lh}^{*[001]} = 0.172$, $m_{lh}^{*[111]} = 0.157$, $m_{lh}^{*[110]} = 0.163$, and $m_{hh}^{*[001]} = 0.46$, $m_{hh}^{*[111]} = 0.56$, $m_{hh}^{*[110]} = 0.53$, experimentally obtained for three orientations of the magnetic field. The obtained energy band parameters and effective masses of the heavy and light holes coincide with those found for bulk Si.

From the width of the CR lines, the average values τ_i were found to be equal to $\tau_{e,1} = 2.28\cdot10^{-10}$ s; $\tau_{e,2} = 3.57\cdot10^{-10}$ s; $\tau_{lh} = 6.9\cdot10^{-10}$ s; $\tau_{hh} = 7.2\cdot10^{-10}$ s, which are by one order of value larger than those obtained in bulk Si. The prolongation of the transport time for photo-excited electrons and holes can be explained by the spatial separation of electrons and holes in the area of

p^+-n junction as well as by reduction of the scattering rate due to the presence of the boron dipole centers.

In contrast to the results obtained in this work, the larger values of effective masses for the heavy holes obtained using optically detected CR in [5] can be explained by the capture of recombined holes at the negative-U dipole boron centers inside δ-shaped barriers confining the ultra-narrow SQW.

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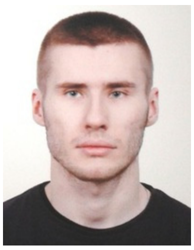

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