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SOLIDS
Electronic Properties

Zeeman Effect for Holes in a Ge/Si System with Quantum Dots

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Abstract—The strong coupling approximation is employed to study the Zeeman effect for the hole ground state in a quantum dot. A method is proposed for calculating the *g* factor for localized states in a quantum dot. This method can be used both for hole states and for electron states. Calculations made for a Ge/Si system with quantum dots prove that the *g* factor of a hole in the ground state is strongly anisotropic. The dependence of the *g* factor on the size of a germanium island is analyzed and it is shown that anisotropy of *g* factor increases with the island size. It is shown that the value of the *g* factor is mainly determined by the contribution of the state with the angular momentum component $J_z = \pm 3/2$ along the symmetry axis of the germanium island. © *2003 MAIK "Nauka/Interperiodica".*

1. INTRODUCTION

The interaction of electronic states having a spin of $\pm 1/2$ with an external magnetic field us described by the Lande *g* factor characterizing the spin splitting of a free electron ($g \approx 2$). The interaction with the lattice potential in solids leads to a considerable difference of the *g* factor from that for a free electron. As the system dimensionality decreases from 3D to 2D and lower, size quantization effects lead to new changes in the *g* factor of charge carriers. For example, quantization for electrons in a low-dimensional system leads to a considerable renormalization of the value of the *g* factor [1] and to its strong anisotropy [2]. The *g* factor contains numerical information on the change in the band structure of the semiconductor upon the reduction in its dimensionality. For this reason, a large number of theoretical and experimental studies are devoted to analysis of this parameter. In some publications dealing with electron states, consistent **kp** theories have been developed, which make it possible to calculate the *g* factor in quantum wells and superlattices [3] as well as in quantum dots [4]. For hole states, the Zeeman effect has been studied theoretically and experimentally for structures with quantum wells [5–7].

Let us describe fundamental differences between two-dimensional quantum wells and quantum dots, which must lead to a change in the *g* factor. Broad quantum wells in magnetic fields of energies smaller than the quantization energy (or the energy of band splitting caused by elastic stresses) can be treated in the approximation of a bulk semiconductor to obtain values of *g* factors for hole subbands directly from the exact form of the 8×8 Hamiltonian in the **kp** theory: $g_\parallel = 6k$, $g_\perp = 0$ for a heavy hole and $g_\parallel = 2k$, $g_\perp = 4k$ for a light hole ($g_\parallel$ and $g_\perp$ are the *g* factor components parallel and perpendicular to the principal axis of the structure (*z* axis); *k* and *q* are the Luttinger parameters, the latter parameter being omitted in view of its smallness). In narrower quantum wells, the indeterminacy in momentum k_z increases, leading to a modification of the *g* factor for a light hole due to admixture of states of the split off band and the conduction band (we assume here that *z* is the growth direction of the epitaxial film) [7]. The Lande factor for a heavy hole at the bottom of the band practically does not change since the heavy hole band does not interact with the nearest bands. In narrow wells, the *g* factors for light and heavy holes change due to the effect of the barriers forming the quantum well [5].

In the case of quantum dots, a considerable renormalization of the *g* factor of hole states must be due to the emergence of a quantizing potential not only to in the growth direction, as in the case of 2D structures, but to equally strong quantization in the lateral direction (in the *xy* plane). This leads to indeterminacy in k_x and k_y and, hence, to a strong mixing of light and heavy hole bands with the split off band [8]. As a rule, this mixing is disregarded in theoretical analysis of the Zeeman effect in 2D systems, since states at the bottom of the band, where k_x, $k_y = 0$, are considered.

In quantum dots created on the basis of stressed heterostructures, the *g* factor may change significantly due to inhomogeneity of strains within quantum dots. If we compare a quantum dot with a quantum well grown in the (100) direction, shear strains ε_{xy}, ε_{xz}, ε_{yz} leading to mixing of light and heavy hole bands are absent in the quantum well [8], while the quantum well experiences such strains.

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Thus, in the case of quantum dots, quantization in all three directions and strain inhomogeneity must lead to a considerable change in the *g* factor of hole states due to energy band mixing.

We propose a method of calculating the *g* factor for hole states in quantum dots, using the strong coupling approach. This method makes it possible to take into account the specific form of a quantizing potential (described not only by an analytic functions) and calculate the *g* factor for a quantum dot of any shape and of an infinitely small size. The proposed method can be also applied for calculating the electron states in quantum dots.

The paper has the following structure. In Section 2, the method of calculating the *g* factor is described. The *g* factor for hole states in germanium quantum dots in a silicon matrix is calculated in Section 3. Strong anisotropy of the *g* factor of holes is discovered and the dependence of the *g* factor of a hole on the quantum dot size is established. The probabilities of Zeeman transitions as functions of the magnetic field direction are investigated. Section 4 is devoted to analysis of obtained results. The factors determining the magnitude of the *g* factor and its dependence on the island size are revealed using a simplified model of noninteracting bands.

2. COMPUTING METHOD

This method is evolution of the idea proposed by us earlier in [9], where an atomistic approach was used for calculating the *g* factor of the hole state in a quantum dot. This approach involves the computation of the angular momentum of a hole in an atomic orbital. However, as we pass to the limiting case of a bulk crystal, this approach fails to provide values matching the bulk value of the *g* factor. For this reason, we extend the former approach by taking into account the angular momentum of Bloch functions.

The Zeeman interaction of a particle having a magnetic moment **M** with a magnetic field **H** can be written in the form

$$\hat{H} = -\hat{\mathbf{M}} \cdot \mathbf{H}.$$

Magnetic moment **M** is connected with angular momentum **J** through the relation

$$\mathbf{M} = g_0 \mu_B \mathbf{J},$$

where μ_B is the Bohr magneton and g_0 is the *g* factor equal to 2 for particles with purely spin electron magnetism and to 1 for those possessing purely orbital electron magnetism.

We introduce the magnetic moment $\mathbf{M}_{QD}$ of a hole (electron) in a quantum dot, which is measured in units of the Bohr magneton:

$$\mathbf{M}_{QD} = \mathbf{L} + 2\mathbf{S},$$

where **L** and **S** are the orbital and spin components of the magnetic moment. We write the Hamiltonian of interaction with the magnetic field in the form

$$\hat{H}_{QD}(\mathbf{H}) = \mu_B \mathbf{H} \cdot \hat{\mathbf{M}}_{QD} = \mu_B (\hat{\mathbf{L}} + 2\hat{\mathbf{S}}) \cdot \mathbf{H}.$$

It follows from symmetry considerations that the ground state in a quantum dot is doubly degenerate and forms a Kramers doublet. The Zeeman interaction energy for states of a Kramers doublet is given by

$$\frac{1}{2}\mu_B \hat{\sigma}_\alpha g_{\alpha\beta} H_\beta,$$

where $\hat{\sigma}_\alpha$ ($\alpha = x, y, z$) are Pauli spin matrices and $g_{\alpha\beta}$ is a tensor which has nine independent components in the general case [10]. In most cases (except in low-symmetry structures), we have $g_{xy} = g_{yx}$, etc., and cross terms can be eliminated by an appropriate choice of the *x*, *y*, and *z* axes (which are known as principal axes). In these axes, the *g* tensor is characterized by three principal values g_{xx}, g_{yy}, and g_{zz}.

In the first order of perturbation theory, the *g* factor can be determined from the solution of a secular equation, which gives

$$|g| = 2\sqrt{\langle \psi | \mathbf{n} \cdot \hat{\mathbf{M}}_{QD} | \psi \rangle^2 + |\langle \psi | \mathbf{n} \cdot \hat{\mathbf{M}}_{QD} | \psi^* \rangle^2|}, \quad (1)$$

where ψ and ψ^* are the wave functions forming a Kramers doublet for a given level and **n** is a unit vector directed along the magnetic field. Consequently, in order to calculate the *g* factor, we must find the matrix elements of operator $\hat{\mathbf{M}}_{QD}$. To determine the matrix elements, we must find wave eigenfunctions ψ and ψ^* for hole or electron states in a quantum dot. We assume that the magnetic field is quite weak and does not change significantly the waves functions of a hole (electron), which enables us to use wave eigenfunctions of the unperturbed Hamiltonian for calculating the matrix elements.

The wave eigenfunctions ψ and ψ^* for hole states were determined by us in [9], where the energy spectrum of holes in a quantum dot was calculated. For this purpose, we used the strong coupling model with basis sp^3 [11]. In this model, each atom is supplied with a set of orbitals *s*, p_x, p_y, and p_z, and the dimensionality of the vector of state of the system is equal to the number of atoms multiplied by the number of orbitals per atom. The interactions between nearest neighbors are taken into account in the two-center approximation [12] as well as the spin–orbit interaction [13]. Deformation effects [14] are taken into account by introducing the dependence of interatomic matrix elements of the Hamiltonian on the orientation of relevant bonds [12] and their length [15]. Vector $|\psi\rangle$ is determined using the free relaxation method [16]. Each vector component ψ_{nN} is the amplitude of probability of finding a particle in the *n*th orbital of the *N*th atom.

Since the vector of the state corresponding to a certain size quantization level is defined as a combination of atomic orbitals, we must determine matrix elements of operator $\hat{\mathbf{M}}_{QD}$ in the representation of atomic orbitals. Let us first define the orbital moment $\mathbf{L}$. We can ascribe to each diagonal matrix element $\langle \psi_{nN}|\hat{\mathbf{L}}|\psi_{nN}\rangle$ the physical meaning of the angular momentum of a particle on the corresponding nth orbital of the chosen Nth atom in a quantum dot.

For a hole (electron) with coordinates (x, y, z) located with probability ψ_{nN}^2 in the nth orbital around the chosen Nth atom with coordinates (X, Y, Z), we can write the angular momentum operator

$$\hat{L}_\alpha = \frac{1}{\hbar} e_{\alpha\beta\gamma}\hat{p}_\beta\hat{r}_\gamma,$$

where $e_{\alpha\beta\gamma}$ is a unit antisymmetric tensor.

Using the rules for differentiating operators with respect to time [17], we can express the momentum operator $\hat{\mathbf{p}} = m\dot{\hat{\mathbf{r}}}$ in terms of Hamiltonian $\hat{H}_0$ and the coordinate operator $\hat{\mathbf{r}}(\hat{x}, \hat{y}, \hat{z})$:

$$\hat{\mathbf{p}} = \frac{im}{\hbar}(\hat{H}_0\hat{\mathbf{r}} - \hat{\mathbf{r}}\hat{H}_0),$$

where m is the mass of a free electron. Then the angular momentum operator has the form

$$\hat{L}_\alpha = \frac{im}{\hbar^2} e_{\alpha\beta\gamma}\hat{r}_\beta\hat{H}_0\hat{r}_\gamma.$$

The obtained expression cannot be used directly for determining the matrix elements $\langle \psi|\hat{\mathbf{M}}_{QD}|\psi\rangle$ and $\langle \psi|\hat{\mathbf{M}}_{QD}|\psi^*\rangle$ since the wave functions ψ and ψ^* have been calculated in the strong coupling approximation, while operator $\hat{\mathbf{r}} = (\hat{x}, \hat{y}, \hat{z})$ of the hole (electron) coordinates is meaningless in this approximation. For this reason, we replace it by coordinate operator $\hat{\mathbf{R}} = (\hat{X}, \hat{Y}, \hat{Z})$ of the atom possessing the orbital,

$$\hat{L}_\alpha = \frac{im}{\hbar^2} e_{\alpha\beta\gamma}\hat{R}_\beta\hat{H}_0\hat{R}_\gamma. \quad (2)$$

Carrying out the substitution $\hat{\mathbf{r}} \longrightarrow \hat{\mathbf{R}}$, we lose a fraction of the angular momentum associated with the strongly oscillating Bloch wave function (which can be referred to as the effective spin angular momentum component) and have only a part of the angular momentum associates with a smooth envelope of the wave function of a hole (electron), viz., orbital component.

If we disregard the interaction between the nearest energy bands, we must simply supplement Eq. (2) with the effective spin component of angular momentum of a charge carrier in the corresponding energy band (conduction band for electrons and valence band for holes) in order to obtain the total moment $\mathbf{M}_{QD}$. However, the state of a hole (electron) in a quantum dot is formed not only by states from the valence (conduction) band; neighboring bands also make a contribution to the formation of the state. The nearest bands for hole states of the split off (SO) band and the conduction band (CB). For electron states, these are bands of heavy holes (HH) and light holes (LH) as well as the split off band. The contribution from other bands is negligibly small.

The wave function of a hole (electron) can be presented in the form

$$|\psi\rangle = |A_1(\mathbf{R})CB\rangle + A_2(\mathbf{R})|HH\rangle + A_3(\mathbf{R})|LH\rangle + A_4(\mathbf{R})|SO\rangle,$$

where coefficients A_1–A_4 depend on the position of an atom in a quantum dot and reflect the contributions from the corresponding bands to the state of a particle in the quantum dot. Each wave function component possesses its own effective spin and interacts with the magnetic field in accordance with the following expressions.

For a hole in the HH band, effective spin $\mathbf{S}_{HH}$ is often introduced for describing Zeeman sublevels [6]: spin $(S_{HH})_z = -1/2$ is ascribed to one of the sublevels with $J_z = -3/2$, while spin $(S_{HH})_z = 1/2$ is ascribed to the other sublevel with $J_z = 1/2$. In this case, the Zeeman interaction can be written in the form

$$\hat{H}(\mathbf{H}) = \mu_B g_{HH}(\hat{\mathbf{S}}_{HH}\cdot\mathbf{H}), \quad (3)$$

where g_{HH} is the g factor for a hole in the HH band. The same can be done for a hole in the LH band: we ascribe spin $(S_{LH})_z = -1/2$ for the sublevel with $J_z = -1/2$ and spin $(S_{LH})_z = 1/2$ for the sublevel with $J_z = 1/2$. Then the Zeeman interaction in the LH band has the form

$$\hat{H}(\mathbf{H}) = \nu_B g_{LH}(\hat{\mathbf{S}}_{LH}\cdot\mathbf{H}), \quad (4)$$

where g_{LH} is the g factor for a hole in the LH band.

For a degenerate valence band, the interaction with the magnetic field at point Γ can be described in the form [8]

$$\hat{H}(\mathbf{H}) = 2\mu_B[k(\hat{\mathbf{J}}\cdot\mathbf{H}) + q(\hat{J}_x^3H_x + \hat{J}_y^3H_y + \hat{J}_z^3H_z)],$$

where J is the effective angular momentum of a hole ($J = 3/2$). We will use this expression in our subsequent analysis, although expressions (3) and (4) can also be used in principle.

The Hamiltonian of the Zeeman interaction in the split off band and in the conduction band can also be expressed in terms of the corresponding effective spins $\mathbf{S}_{SO}$ and $\mathbf{S}_{CB}$. For a hole in the split off band, we have

$$\hat{H}(\mathbf{H}) = \mu_B g_{SO}(\hat{\mathbf{S}}_{SO}\cdot\mathbf{H}), \quad (5)$$

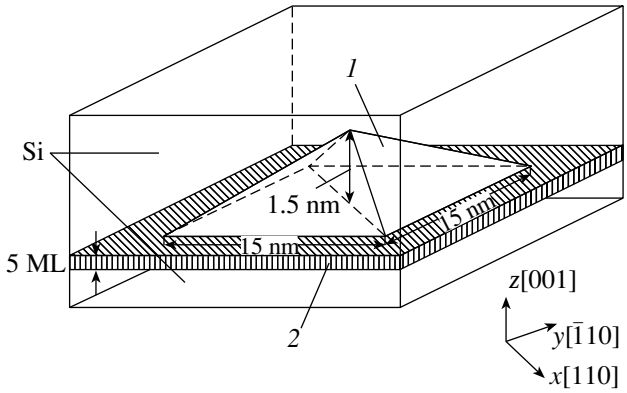

Fig. 1. Schematic diagram of a typical quantum dot (germanium island) in silicon: germanium island (quantum dot) (*1*), germanium film (wetting layer) (*2*), and monolayer (ML).

while for an electron in the conduction band, we have

$$\hat{H}(\mathbf{H}) = \mu_B g_{CB}(\hat{\mathbf{S}}_{CB} \cdot \mathbf{H}), \tag{6}$$

where g_{SO} is the g factor of a free hole in the split off band, g_{CB} is the g factor in the conduction band, and effective spin operators $\hat{\mathbf{S}}_{SO}$ and $\hat{\mathbf{S}}_{CB}$ are defined in terms of the Pauli spin matrices $\hat{\sigma}_x$, $\hat{\sigma}_y$, and $\hat{\sigma}_z$, acting on the corresponding spin variables, $\hat{S}_\alpha = \hat{\sigma}_\alpha/2$.

The total energy of interaction with the magnetic field taking into account the orbital moment **L** is given by the sum

$$\begin{aligned}\hat{H}(\mathbf{H}) &= 2\mu_B[k(\hat{\mathbf{J}} \cdot \mathbf{H}) \\ &+ q(\hat{J}_x^3 H_x + \hat{J}_y^3 H_y + \hat{J}_z^3 H_z)] \\ &+ \mu_B g_{SO}(\hat{\mathbf{S}}_{SO} \cdot \mathbf{H}) + \mu_B g_{CB}(\hat{\mathbf{S}}_{CB} \cdot \mathbf{H}) + \mu_B(\hat{\mathbf{L}} \cdot \mathbf{H}),\end{aligned} \tag{7}$$

where $\hat{\mathbf{L}}$ is defined by formula (2). It follows hence that

$$\begin{aligned}(\hat{M}_{QD})_\alpha &= 2k\hat{J}_\alpha + 2q\hat{J}_\alpha^3 \\ &+ g_{SO}(\hat{S}_{SO})_\alpha + g_{CB}(\hat{S}_{CB})_\alpha + \hat{L}_\alpha.\end{aligned} \tag{8}$$

The final formula for calculating the total magnetic moment has the form

$$\begin{aligned}(\hat{M}_{QD})_\alpha &= 2k\hat{J}_\alpha + 2q\hat{J}_\alpha^3 + g_{SO}(\hat{S}_{SO})_\alpha \\ &+ g_{CB}(\hat{S}_{CB})_\alpha + \frac{im}{\hbar} e_{\alpha\beta\gamma}\hat{R}_\beta \hat{H}_0 \hat{R}_\gamma.\end{aligned} \tag{9}$$

Using now this expression, we can determine the matrix elements $\langle \psi | \hat{\mathbf{M}}_{QD} | \psi \rangle$ and $\langle \psi | \hat{\mathbf{M}}_{QD} | \psi^* \rangle$ and calculate the g factor by formula (1).

3. CALCULATION OF THE g FACTOR IN A Ge/Si SYSTEM WITH QUANTUM DOTS

Quantum dots in a Ge/Si system are formed during heteroepitaxy of germanium on a Si(100) substrate under certain conditions of transition from the 2D-layer mechanism of germanium film growth to the 3D growth. A typical size of islands in the familiar experimental studies varied from 10 to 20 nm, their height being 1–2 nm; consequently, the behavior of charge carriers in these islands is determined by quantum size effects [18]. The gap in energy bands existing in the Ge/Si heterosystem and deformation effects lead to the formation of a potential well in germanium for holes only. The states in a quantum dot are mainly formed from the states of the valence band, i.e., are a superposition of states $|3/2, \pm 3/2\rangle$, $|3/2, \pm 1/2\rangle$, and $|1/2, \pm 1/2\rangle$ (state $|J, J_z\rangle$ is characterized by the angular momentum J and its component J_z along the z axis, viz., growth direction; Fig. 1). It follows from experimental results that a germanium island can be regarded as a square pyramid whose height h is an order of magnitude smaller than the base side l ($h/l \sim 1/10$) [19]. In fact, an island is a quasi-two-dimensional quantum object with a preferred symmetry axis z. The strain distribution in a quantum dot [14] removes the degeneracy existing at point Γ in the valence band. Since the crystal is subjected to uniaxial extension along the z axis within the island, states $|3/2, \pm 3/2\rangle$ of heavy holes are at the bottom of the valence band [20]. Consequently, we can expect that the contribution from heavy holes to the ground state in a quantum dot is predominant. The same conclusion can be drawn taking into account the fact that the effective mass of heavy holes is larger than that of light holes.

Let us consider the case when the magnetic field is parallel to the growth direction ($\mathbf{H} \parallel z$). The energy of interaction with the field is determined by the magnetic moment component along the magnetic field, i.e., along z. In order to calculate the g factor, we must know the matrix elements of operators $\hat{J}_z$, $\hat{J}_z^3$, $(\hat{S}_{SO})_z$, $(\hat{S}_{CB})_z$, and $\hat{L}_z$.

Let us first demonstrate that g factor can be estimated only from the wave function expansion in the basis $|J, J_z\rangle$, i.e., in the basis $|3/2, \pm 3/2\rangle$, $|3/2, \pm 1/2\rangle$, and $|1/2, \pm 1/2\rangle$. We will disregard the effect of the conduction band on the hole states in the Ge/Si system of a quantum dot because the contribution from the states of this band to the wave function amounts to only about 0.5%.

The results of expansion of the wave function of the ground state in a quantum dot having a size $l = 15$ nm and $h = 1.5$ nm are compiled in the table. The component with $J_z = \pm 3/2$ constitutes approximately 84% of the entire wave function. The remaining part corresponds to the component with $J_z = \pm 1/2$. It can be seen from the table that the state with the "up" spin, $|\uparrow\rangle$ (the state with the average angular momentum directed

Results of expansion of wave functions in the basis $|J, J_z\rangle$ for two spin sublevels $|\uparrow\rangle$ and $|\downarrow\rangle$ of the ground state in a germanium island of height $h = 1.5$ nm and base side $l = 15$ nm

$\lvert J, J_z\rangle$	$\lvert\frac{3}{2}, \frac{3}{2}\rangle$	$\lvert\frac{3}{2}, \frac{1}{2}\rangle$	$\lvert\frac{3}{2}, -\frac{1}{2}\rangle$	$\lvert\frac{3}{2}, -\frac{3}{2}\rangle$	$\lvert\frac{1}{2}, \frac{1}{2}\rangle$	$\lvert\frac{1}{2}, -\frac{1}{2}\rangle$
$\lvert\uparrow\rangle$	83.67%	2.26%	4.7%	0.08%	1.17%	8.11%
$\lvert\downarrow\rangle$	0.08%	4.7%	2.26%	83.67%	8.12%	0.67%

along the field) is mainly formed from components with $J_z = 3/2$ and $J_z = -1/2$, while the $|\downarrow\rangle$ state (the state with the average angular momentum opposite to the field) is formed by components with $J_z = -3/2$ and $J_z = 1/2$. The component with $J_z = \pm 1/2$ reflects contributions from states$|3/2, \pm 1/2\rangle$, $|1/2, \pm 1/2\rangle$, these contributions being almost identical and constituting about 8% each. This means that the formation of the ground state in a quantum dot is equally affected by the light hole subband and the split off subband.

If the ground state of a hole in a quantum dot were formed only by states with $J_z = \pm 3/2$, i.e., the $|\uparrow\rangle$ state corresponded to $J_z = 3/2$ and the $|\downarrow\rangle$ state to $J_z = -3/2$, the Zeeman splitting in a magnetic field $\mathbf{H} \parallel z$ would be determined by the expression

$$\begin{aligned} E(H_z) &= 2\mu_B \langle (M_{QD})_z \rangle H_z \\ &= 2\mu_B H_z \left(2k\frac{3}{2} + 2q\frac{27}{8} + \langle L_z \rangle \right), \end{aligned} \tag{10}$$

where $\langle (M_{QD})_z \rangle$ and $\langle L_z \rangle$ are the mean values of the z components of the magnetic and orbital moments in the $|\uparrow\rangle$ state.

In obtaining estimates, the term with q can be omitted in view of its smallness ($|q| = 0.06$) [21]. If we take into account the admixture of states with $J_z = \pm 1/2$, expression (10) is transformed to

$$\begin{aligned} E(H_z) &= 2\mu_B H_z \left\{ 2k(a-d)\frac{3}{2} \right. \\ &\left. + [2k(b-c) + g_{SO}(e-f)]\frac{1}{2} + \langle L_z \rangle \right\}, \end{aligned}$$

where a, b, c, and d are the probabilities of values $J_z = 3/2$, $J_z = 1/2$, $J_z = -1/2$, and $J_z = -3/2$ (for $J = 3/2$) in the $|\uparrow\rangle$ state, respectively, e and f are the probabilities of the values $J_z = 1/2$ and $J_z = -1/2$ (for $J = 1/2$) in the $|\uparrow\rangle$ state, respectively. For a quantum dot of size $l = 15$ nm and $h = 1.5$ nm, $a \approx 0.84$, $b \approx 0.02$, $c \approx 0.05$, $d \approx 0$, $e \approx 0.01$, and $f \approx 0.08$ (see table).

An estimate obtained disregarding the $\langle L_z \rangle$ term gives the following value for the g factor:

$$g_{zz} \approx 6k \times 0.82 - 2k \times 0.03 + g_{SO} \times 0.07,$$

here, $k = -3.41 \pm 0.03$ [21] and $g_{SO} = -10 \pm 3$ [22], which gives $|g_{zz}| \approx 15.86$.

Calculating the g factor by formula (1) for the same island size taking into account the orbital moment $\langle L_z \rangle$ and using the wave functions determined in the strong coupling approximation, we obtain $|g_{zz}| = 15.71$.

A comparison with the bulk value of the longitudinal g factor for a heavy hole, $|g_{HH}| \approx 6k = 20.46$, shows that size quantization reduces the g factor, indicating the suppression of the spin-orbit interaction due to an admixture of the state with a smaller value of J ($J = 1/2$) and a decrease in the effective angular momentum of the particle.

In order to estimate the contribution of the orbital moment, we calculated g factor using formulas (1) and (8), omitting in Eq. (8) all the terms except $\hat{L}_\alpha$. As a result, we obtained an order-of-magnitude smaller value of g factor: $|g_{zz}| = 0.59$. Thus, the g factor is mainly determined by the effective angular momentum **J** rather than by the orbital moment **L**.

We will give here the principal values of the g factor for the ground state in a quantum dot of size $l = 15$ nm and $h = 1.5$ nm, calculated by formula (1): $|g_{zz}| = 15.71$ (in the growth direction [001]), $|g_{xx}| = 1.14$ (in the [110] direction), and $|g_{yy}| = 1.76$ (in the $[\bar{1}\,10]$ direction).

3.1. Dependence of g Factor on the Size of Germanium Island

The obtained results clearly demonstrate anisotropy in the values of g factor: g_{zz} is an order of magnitude larger than the values of g_{xx} and g_{yy}. Anisotropy increases upon an increase in the island base for a constant height (Fig. 2). This tendency can be explained by the fact that the wave function of the ground state is close in composition to the wave function $|3/2, \pm 3/2\rangle$ (for a heavy hole), in which the transverse components of the g factor are close to zero [6].

We can assume that the wave function of the ground state becomes closer and closer to the wave function of a heavy hole as the size of the island increases, which enhances the anisotropy of the g factor.

Indeed, according to the results of our calculations, the contribution of the state with $J_z = \pm 3/2$ to the wave function of a hole increases with the lateral dimension

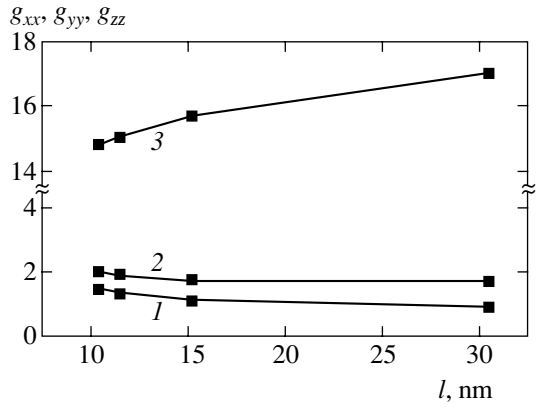

Fig. 2. Dependence of the g factor of the ground state of a hole on the lateral size l of a germanium island of height h = 1.5 nm: g_{xx} (*1*), g_{yy} (*2*), and g_{zz} (*3*).

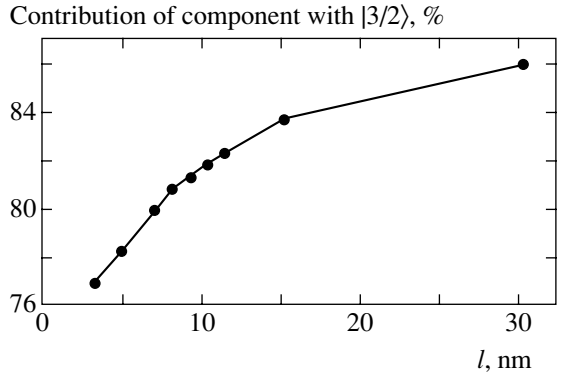

Fig. 3. Contribution of the component with $J_z = \pm 3/2$ to the wave function of the ground state of a hole as a function of the lateral size l of a germanium island of height h = 1.5 nm.

of the island, and the wave function tends to "pure" state $|3/2, \pm 3/2\rangle$ (Fig. 3). For example, as the lateral size l of the island increases from 15 to 30 nm for height h = 1.5 nm, the contribution from the component with $J_z = \pm 3/2$ to the wave function of the ground state increases from 83 to 86%. Anisotropy of the g factor increases: the value of $|g_{zz}|$ increases to 17.0, while the transverse components decrease to $|g_{xx}| = 0.91$ and $|g_{yy}| = 1.71$. If we increase the island size to that the pyramid proportion is preserved ($h/l = 1/10$), the anisotropy of the g factor becomes stronger. For example, for l = 30 nm and h = 3 nm, the principal values of the g factor are as follows: $|g_{zz}| = 20.99$, $|g_{xx}| = 0.06$, and $|g_{yy}| = 1.1$. It turns out that the contribution of the component with $J_z = \pm 3/2$ to the wave function of the ground state in this case increases to 90%, leading to such a strong anisotropy.

The obtained dependence of the g factor on the island size indicates the correctness of our approach. Indeed, as the lateral size of the island increases, we pass to the limiting case of a pseudomorphic stressed germanium film. Inhomogeneity of strains typical of quantum dots disappears. The indeterminacy in k_x and k_y for states at the bottom of the band becomes equal to zero. All these factors suppress the interaction of the HH band with other energy bands; as a result, the g factor of the ground state tends to the g factor of a heavy hole, which is in accordance with our results.

3.2. Sharpness of Germanium Island Boundaries

The above values of g factor were obtained for an island with sharp boundaries. If we take into account diffuse blurring of the island boundaries, which is always observed in real Ge island, these values will slightly change.

The blurring of boundaries was taken into account as follows: each atom in the crystal lattice was replaced, with a probability of 2/3, by one of its four nearest neighbors. As a result, we obtained a boundary with a smooth variation in the composition of the substance within three monolayers.

Taking into account the blurring of island boundaries, we found that the transverse components of the g factor change significantly (e.g., the value of $|g_{xx}|$ decreases from 1.14 to 0.52 for an island with a lateral size of l = 15 nm, while the value of $|g_{yy}|$ decreases from 1.76 to 0.18. The longitudinal component $|g_{zz}|$ of the g factor virtually does not change and amounts to 15.81. Consequently, anisotropy of the g factor increases on account of blurring of the heteroboundary. This is probably associated with an effective increase in the island size.

3.3. Probability of Zeeman Transitions

The probability of Zeeman transitions is directly connected with the form of the wave function. For a state with $J_z = \pm 3/2$ in a magnetic field $\mathbf{H} \parallel z$, induced transitions between the Zeeman subleves with $J_z = 3/2$ and $J_z = -3/2$ are forbidden by the selection rules since allowed transitions must satisfy the condition $\Delta J_z = \pm 1$. An admixture of a state with $J_z = \pm 1/2$ facilitates transitions between the Zeeman sublevels of the ground state in a germanium island. Consequently, the prohibition imposed on Zeeman transition is released upon an increase in the island size.

For an arbitrary direction $\mathbf{h}$ of the magnetic field, the energy of interaction with the field is determined by the angular momentum component along $\mathbf{h}$. States $|J, J_z\rangle$ are transformed into states $|J, J_h\rangle$ as follows:

$$|J, J_z\rangle \longrightarrow |J, J_h\rangle = \sum_{J_z} R^J_{J_z J_h}(\theta, \varphi)|J, J_z\rangle,$$

here, θ and φ are polar angles of vector $\mathbf{h}$ in the system of coordinates x, y, z, and matrix R is connected with the standard matrix of rotations [23],

$$R^J_{J_z J_h}(\theta, \varphi) = D^J_{J_z J_h}(0, -\theta, -\varphi).$$

In a particular case when $\theta = \pi/2$ and $\varphi = 0$, the magnetic field direction lies in the plane of the island and coincides with the x axis. Let us consider a pure state with $J_z = 3/2$. In the $|J, J_z\rangle$ representation, the wave function of this state can be written in the form

$$|\psi\rangle = a\left|\frac{3}{2}, \frac{3}{2}\right\rangle + b\left|\frac{3}{2}, \frac{1}{2}\right\rangle + c\left|\frac{3}{2}, -\frac{1}{2}\right\rangle + d\left|\frac{3}{2}, -\frac{3}{2}\right\rangle = \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix},$$

where the squares of the coefficients (a^2, b^2, c^2, and d^2) reflect contributions from the states with corresponding values of J_z ($a^2 + b^2 + c^2 + d^2 = 1$). Under transformation $R^J_{J_z J_h}(\pi/2, 0)$, state $\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$ is transformed into $\begin{pmatrix} \sqrt{1/8} \\ \sqrt{3/8} \\ \sqrt{3/8} \\ \sqrt{1/8} \end{pmatrix}$. It follows hence that the fraction of each component with $J_h = \pm 1/2$ amounts to 3/8 of the entire wave function. In the whole, they constitute 75%; i.e., the contributions from components with $J_h = \pm 1/2$ for the direction of magnetic field **H** in the basal plane of the are larger as compared to the case when **H** $\parallel z$, and the probability of Zeeman transitions increases. This is also observed in the case when the wave function initially contains a correction with $J_z = \pm 1/2$ as, for example, for the ground state in the quantum dot in question, where is amounts to 16%.

Let us consider some numerical estimates of the probabilities of Zeeman transitions for different directions of the magnetic field.

The probability of an induced transition between Zeeman sublevels is determined by the interaction of the magnetic moment with oscillating magnetic microwave field $H_\perp \cos(2\pi\nu t)$ (field $H_\perp$ is perpendicular to the constant magnetic field) and is proportional to the squared matrix element of the magnetic moment component $\mu_\perp$ of a particle in the direction of this field [24],

$$P_{\uparrow\downarrow} \sim |\langle\downarrow|\hat{\mu}_\perp H_\perp|\uparrow\rangle|^2.$$

If the magnetic field direction is such that **H** $\parallel z$ the magnetic moment component $\mu_\perp$ lies in the island basal plane and is proportional to the principal values of the g tensor, g_{xx} (direction [110]) and g_{yy} (direction $[\bar{1}10]$). In the particular case when the microwave field $H_\perp$ is directed along [110], the transition probability $P_{\uparrow\downarrow}$ is proportional g^2_{xx}.

If the direction of the constant magnetic field is such that **H** $\perp z$, the magnetic moment component lies in the plane perpendicular to the basal plane; in the particular case, when the microwave field $H_\perp$ is directed along [100], this component is proportional to the principal value of the g tensor: $\mu_\perp \propto g_{zz}$. In this case, the transition probability is $P_{\uparrow\downarrow} \propto g^2_{xx}$.

It can be seen that, for $g_{zz} = 15.71$, $g_{xx} = 1.14$, and $g_{yy} = 1.76$, the probabilities of induced transitions for two directions of the magnetic field (**H** $\parallel z$ and **H** $\perp z$) differ approximately by two orders of magnitude. If, in addition, we take into account a decrease in the transverse components of the g factor due to blurring of the boundaries ($g_{xx} = 0.52$ and $g_{yy} = 0.18$), the difference in the transition probabilities for **H** $\parallel z$ and **H** $\perp z$ will be by more than three orders of magnitude.

4. DISCUSSION

The obtained results show that the main factor determining the dependence of the g factor on the size of an island is the change in the contribution to the wave function of a hole from the component with $J_z = \pm 3/2$ upon a change in the island size.

The factors determining the relation between the contributions from the components with $J_z = \pm 3/2$ and $\pm 1/2$ can be grasped from the following simplified model disregarding the interaction between energy bands. Let us consider separately the quantization of the energy spectra of holes with $J_z = \pm 3/2$ and $J_z = \pm 1/2$. In such a model, the deepest energy levels belong to holes with $J_z = \pm 3/2$; in the range of excited states, these levels are mixed with the levels of holes with $J_z = \pm 1/2$. In a more realistic model taking into account the interaction between energy bands (e.g., the six- or eight-band kp model or the strong coupling model), the energy range containing energy levels of holes with $J_z = \pm 1/2$ and $\pm 3/2$ also contains some "mixed" states with comparable contributions from both types of holes, while the range corresponding to the deepest layers contains states formed mainly by holes with $J_z = \pm 3/2$. Such a qualitative model is in agreement with the results of our calculations.

Figure 4 shows the contribution from the component with the momentum component $J_z = \pm 3/2$ to the wave functions of states in a quantum dot of size l = 15 nm and h = 1.5 nm. The results of expansion show that the component with $J_z = \pm 3/2$ constitutes approximately 84% of the wave function of the ground state (E_0 = 420 meV). For the first excited state (E_1 = 377), the contribution from the component with v decreases approximately to 79%. As the number of the excited state increases, a tendency towards a decrease in the

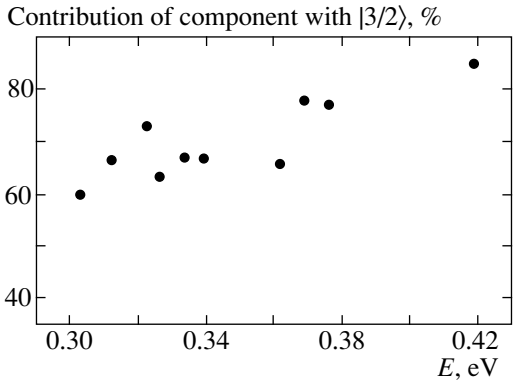

Fig. 4. Contribution of the component with $J_z = \pm 3/2$ to the states of the discrete spectrum of a germanium island. The energy of the state measured from the edge of the valence band of silicon is laid along the abscissa axis. The island size: height $h = 1.5$ nm and base side $l = 15$ nm.

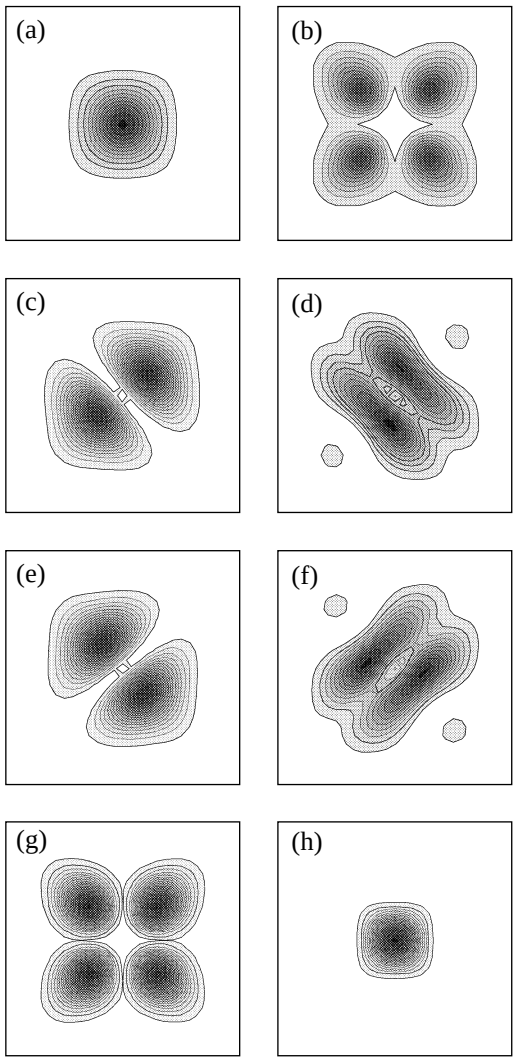

Fig. 5. Wave function density distribution for the component with $J_z = \pm 3/2$ (a, c, e, and g) and $J_z = \pm 1/2$ (b, d. f, and h) (projection on the plane of the pyramid base) in the ground (a, b), first excited (c, d), second excited (e, f), and third excited (g, h) states of a hole in a quantum dot.

component with $J_z = \pm 3/2$ is observed. For the ninth excited state ($E_9 = 303$ meV), the contribution from the component with $J_z = \pm 3/2$ amounts approximately to 60%.

The form of the wave function of the ground state is determined by the separation between the ground energy level and the states of holes with $J_z = \pm 3/2$, which lie in the range of excited states in a quantum dot.

The data presented in Fig. 4 show that the dependence of the contribution from the component with $J_z = \pm 3/2$ on the hole energy cannot be described by a smooth function. In order to explain the step form of this dependence, we analyzed the form of wave functions separately for the components with $J_z = \pm 3/2$ and $\pm 1/2$. Figure 5 shows the wave functions for the components with $J_z = \pm 3/2$ and $\pm 1/2$, forming the first four states in the quantum dot. In the ground state, the component with $J_z = \pm 3/2$, which constitutes 84%, is *s*-shaped. However, the component with $J_z = \pm 1/2$, which is admixed on account of interaction between energy bands and constitutes approximately 16%, is *d*-shaped. If we return to the simplified model and consider separately the quantization of the spectra of holes with $J_z = \pm 3/2$ and $\pm 1/2$, each of these two spectra contain *s*-, *p*-, and *d*-shaped states, etc. (see Fig. 6). Naturally, the *s*-shaped state will be the lowest state in both spectra, followed by *p*- and *d*-shaped states, etc. The admixture of a state with $J_z = \pm 1/2$ to a state with $J_z = \pm 3/2$ is inversely proportional to the difference in the energies of these states, i.e., $(E_{\pm 3/2} - E_{\pm 1/2})^{-1}$. It follows from the data presented in Fig. 5 that the *s* state from the spectrum of a hole with $J_z = \pm 3/2$ interacts with the *d* state from the spectrum of a hole with $J_z = \pm 1/2$ during the formation of the ground energy level. In this case, the contribution from the component with $J_z = \pm 1/2$ is determined by the energy gap $\Delta E_0 = E^s_{\pm 3/2} - E^d_{\pm 1/2}$. During the formation of the first and second excited states, the *p* state from the spectrum of a hole with $J_z = \pm 3/2$ interacts with the *p* state of a hole with $J_z = \pm 1/2$. In such cases, the energy gaps $\Delta E_1 = \Delta E_2 + E^p_{\pm 3/2} - E^p_{\pm 1/2}$ coincide; consequently, the contributions from the component with $J_z = \pm 1/2$ are practically identical. During the formation of the third excited state, *d* states from the spectrum of a hole with $J_z = \pm 3/2$ interact with the *s* state from the spectrum of a hole with $J_z = \pm 1/2$. In this case, the contribution from the component with $J_z = \pm 1/2$ is determined by the energy gap $\Delta E_3 = E^d_{\pm 3/2} - E^s_{\pm 1/2}$; i.e., the separation between interacting energy levels decreases sharply, and the contribution from the component with $J_z = \pm 1/2$ increases significantly. Thus, we can establish a relation between the energy gaps in all the four cases ($\Delta E_0 > \Delta E_1$, $\Delta E_1 = \Delta E_2$, and $\Delta E_2 > \Delta E_3$) and explain the dependence of the contribution of

the component with $J_z = \pm 1/2$ on the number of the state in a discrete spectrum in a quantum dot.

The interpretation for the next energy levels is complicated on account of the fact that the wave functions of these states have a complex form and cannot be classified as *s*-, *p*-, … shaped states.

Let us now consider the factors determining the variation of the relation between the contributions of components with $J_z = \pm 1/2$ and $\pm 3/2$ upon the variation of the island size.

If the size of an island increases so that the proportions between dimensions is preserved ($h/l = 1/10$), the distribution and magnitude of strains in the island does not change significantly; consequently, the splitting between the HH and LH bands remains unchanged. The size quantization energy decreases and amounts, for example, to a few millielectronvolts for $l = 100$ nm and $h = 10$ nm. As a result, the ground state in the spectrum of a hole with $J_z = \pm 3/2$ shifts towards the bottom of the potential well. Excited states are less sensitive to a change in the island size since their localization radius is larger, and the wave functions penetrate more strongly under the barrier (to silicon surrounding the germanium island). Consequently, the position of energy levels for holes with $J_z = \pm 1/2$ changes weaker than for holes with $J_z = \pm 3/2$ upon an increase in the island size. For this reason, the energy gap ΔE_0 between the ground *s* state of a hole with $J_z = \pm 3/2$ and the *d* state of a hole with $J_z = \pm 1/2$ increases. Accordingly, the contribution from the component with $J_z = \pm 1/2$ to the ground state of the hole decreases, and the wave function becomes closer to the state of a hole with $J_z = \pm 3/2$. In this case, the main factor determining the change in the relation between the components with $J_z = \pm 3/2$ and $\pm 1/2$ is a quantum size factor (decrease in the size quantization energy).

If only the lateral size of the island increases, the size quantization energy remains practically unchanged since it is mainly determined by the height of the island. However, an increase in the l/h ratio leads to an increase in biaxial strain $\varepsilon_{zz} - (\varepsilon_{xx} + \varepsilon_{yy})/2$ [25], leading to an increase in the splitting between the HH and LH subbands. In this case, the reason for increasing the energy gap ΔE_0 is a deformation factor (change in strains in the island).

The experimental value of the *g* factor for a hole in quantum dots is usually a result of indirect measurements. As a rule, the photoluminescence spectrum in a magnetic field is analyzed [26–28], and the *g* factor of a hole is calculated from the experimentally determined *g* factor of an exciton (g_{ex}) and the *g* factor of an electron (g_e) using the relation $g_{ex} = g_{HH} \pm g_e$ (the minus sign is used for optically active excitons and the plus sign, for optical inactive excitons). In order to eliminate an additional systematic error associated with the existence of exchange interaction between the electron and the hole in an exciton, a solitary hole in a quantum dot must be analyzed instead of a hole bound with an electron to form an exciton complex. For this purpose, an experiment involving tunneling of a hole through a quantum dot in a magnetic field, similar to that proposed in [29] for an electron, can be made. In this case, it is important to choose appropriately the magnetic field direction since it determines to a considerable extent the Zeeman splitting and the intensity of the Zeeman transitions. For the $\mathbf{H} \parallel z$ direction, Zeeman transitions are virtually forbidden. For $\mathbf{H} \perp z$, the Zeeman splitting is small. For this reason, it is expedient to carry out experiments in a tilted magnetic field, when the Zeeman splitting is strong enough, and the intensity of induced transition is appreciable.

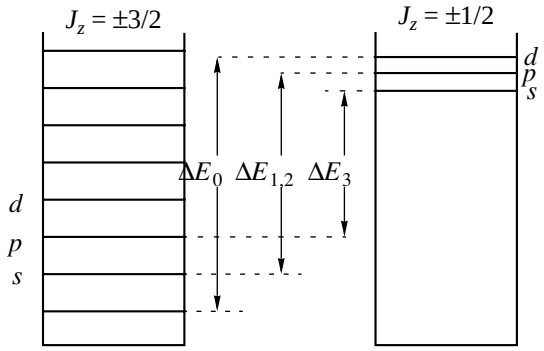

Fig. 6. Schematic diagram of the energy spectra of holes with $J_z = \pm 3/2$ in the simplified model of noninteracting energy bands. The spectra are separated in space. Letters *s*, *p*, and *d* mark the energy levels corresponding to *s*-, *p*- and *d*-shaped states.

The method of calculating the *g* factor in quantum dots proposed here will make it possible to compare consistently the theory and available experimental data on *g* factors of hole (electron) states in quantum dots grown in various heterosystems, since its applicability is not limited to quantum dots in the Ge/Si system.

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