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Ge/Si Quantum Dots in External Electric and Magnetic Fields

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Abstract—Electric field-induced splitting of the lines of exciton optical transitions into two peaks is observed for Ge/Si structures with quantum dots (QDs). With increasing field, one of the peaks is displaced to higher optical transition energies (blue shift), whereas the other peack is shifted to lower energies (red shift). The results are explained in terms of the formation of electron–hole dipoles of two types differing in the direction of the dipole moment; these dipoles arise due to the localization of one electron at the apex of the Ge pyramid and of the other electron under the base of the pyramid. By using the tight-binding method, the principal values of the g factor for the hole states in Ge/Si quantum dots are determined. It is shown that the g factor is strongly anisotropic, with the anisotropy becoming smaller with decreasing QD size. The physical reason for the dependence of the g factor on quantum-dot size is the fact that the contributions from the states with different angular-momentum projections to the total wave function change with the QD size. Calculations show that, with decreasing QD size, the contribution from heavy-hole states with the angular-momentum projections ±3/2 decreases, while the contributions from light-hole states and from states of the spin-split-off band with the angular-momentum projections ±1/2 increase. *© 2004 MAIK "Nauka/Interperiodica".*

1. QUANTUM DOTS IN AN ELECTRIC FIELD

Application of an electric field to a system of quantum dots (QDs) results in energy-level shifts in optical transitions (the Stark effect in quantum-confinement systems; see, e.g., [1, 2]). Most studies of the Stark effect have been performed on type-1 (InAs/GaAs) heterostructures. The red shift of optical transition energies in an electric field was observed in those studies. In type-2 heterostructures, electrons and holes are localized on different sides of the heterointerface and, once their spatial separation is sufficiently large, one may expect a strong manifestation of the Stark effect.

The Ge/Si structures with QDs form type-2 heterojunctions. When an electron–hole pair is photogenerated, the hole is localized in Ge, whereas the electron is located in the potential well formed in Si near the vertex of the Ge pyramid. Such an excitation is called the spatially indirect exciton. If a biexciton is formed, holes still remain localized in Ge; however, for the second electron, localization under the base of the Ge pyramid appears to be energetically more favorable [3]. Such a geometrical configuration results in opposite orientations of the dipoles with respect to the electric field directed along the symmetry axis of the Ge pyramid (along the growth axis; Fig. 1).

Interband optical transitions in Ge/Si systems with QDs in an electric field were studied in [4] using photocurrent spectroscopy. Two conditions have to be satisfied for experimental observation of the Stark effect. First, the size of Ge nanocrystals must be sufficiently small for the spectrum of electronic states to be discrete. The other condition is that the spatial electron–hole separation must be such that the electric dipole moments are sufficiently large. To satisfy these conditions, the method of heteroepitaxy of Ge on Si with the addition of oxygen before Ge deposition was developed in [4]. This method provides the possibility of forming hemispherical Ge islands with a size of the base of the nanocluster of about 6 nm and a height of 3–4 nm.

The electric field ranged up to 100 kV/cm. For low electric fields, a symmetric photocurrent peak is observed at a photon energy of about 1040 meV for the structures studied; this peak is attributed to indirect excitonic transitions between the hole ground state in Ge and the ground state of an electron localized in Si near the Ge/Si heterointerface. An electron–hole pair generated by photoexcitation dissociates into its components due to thermal fluctuations (the measurements are made at room temperature) and contributes to the photocurrent. The width of the photocurrent peak increases with electric field, and, finally, the peak splits into two peaks. As the electric field is increased further, the energy positions of these two peaks are displaced in opposite directions (the red and blue shifts; Fig. 2).

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These results have a sufficiently simple qualitative explanation in terms of the conception of the two dipoles that are formed on Ge quantum dots and have opposite directions with respect to the applied electric field. For one of the dipoles, the external field increases the overlap of the wave functions of the electron and the hole and, therefore, increases the exciton binding energy and gives rise to a blue shift in the photocurrent spectrum. For the dipole of the opposite direction, the overlap of the wave functions decreases, thereby producing a decrease in the exciton binding energy and a red shift of the photocurrent peak.

Perturbation-theory estimations of the spatial separations between electrons and holes and the experimental data on the electric-field dependence of the photocurrent peaks yield values that agree with the geometrical QD configuration obtained by electron microscopic studies.

2. QUANTUM DOTS IN A MAGNETIC FIELD

A splitting of discrete levels of an atom or a QD (artificial atom) in a magnetic field (Zeeman effect) is determined by the magnetic-moment projection on the field direction. In turn, the magnetic moment is related to the angular momentum by the Lande factor, which actually determines the value of the splitting of discrete levels. The Lande splitting factor for a free electron (≈2) describes the interaction of the electronic ±1/2 spin states with an external magnetic field. In solids, the *g* factor is substantially different from the *g* factor for free electrons due to the interaction with the lattice potential. With lowering the dimensionality of the system from the three-dimensional (3*D*) to the two-dimensional (2*D*) case and further, the quantum-confinement effects also change the carrier *g* factor. For example, for electrons in low-dimensional systems, the quantization results in substantial renormalization of the value of the *g* factor [5] and in its strong anisotropy [6]. The Lande factor contains quantitative information on the change in the semiconductor band structure with decreasing dimensionality and has been studied in numerous experimental and theoretical papers. For electron states, there are papers in which the *g* factor of an electron in a quantum well or a QD was calculated [7]. For hole states, the Zeeman effect has been studied theoretically and experimentally for structures with quantum wells.

In the case of QDs, the existence of confinement potential not only in the growth direction (as in the case of 2*D* structures) but also an equally strong quantization in the lateral direction should produce a significant renormalization of the *g* factor for hole states. In addition, for QDs in strained heterostructures, nonhomogeneity of strains inside quantum dots also strongly affects the *g* factor. Comparison of a quantum dot and a quantum well, both grown in the ⟨100⟩ direction, shows that in the latter structure there are no shear strains ε_{xy},

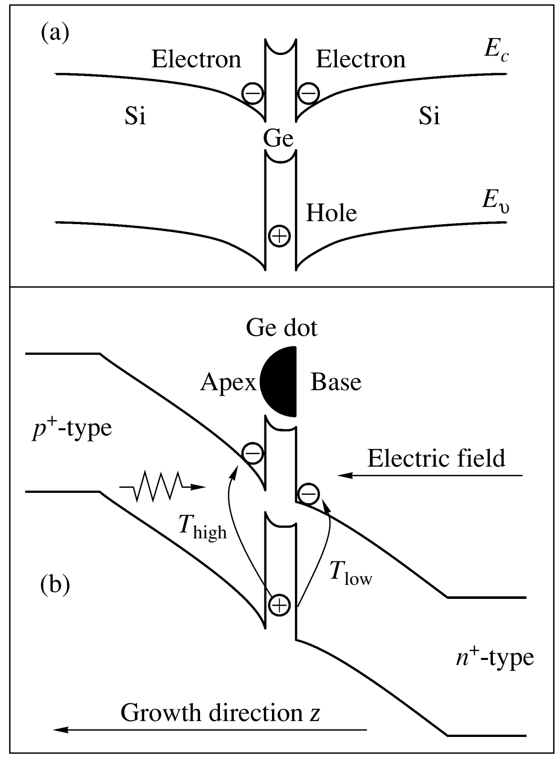

Fig. 1. (a) Band structure of the Ge/Si type-2 heterostructure along the growth direction passing through the center of symmetry of a Ge quantum dot and (b) band structure of the *p*–*i*–*n* diode under reverse bias (schematic).

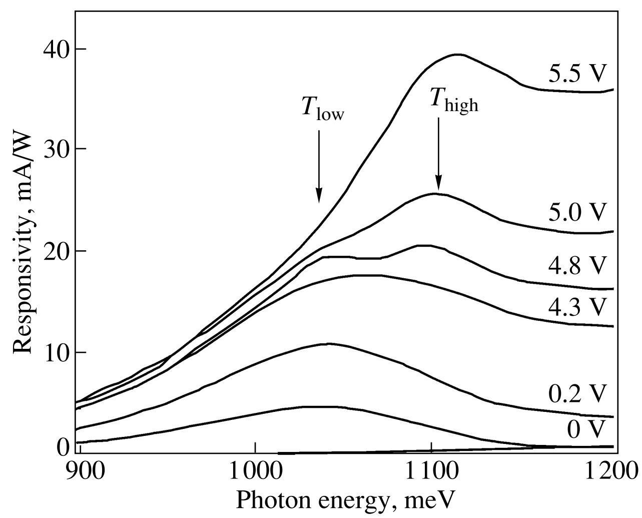

Fig. 2. Dependence of photocurrent spectra on reverse bias.

ε_{xz}, and ε_{yz} (here, **z** is the growth direction and **x** and **y** lie in the base plane of the pyramid), resulting in mixing of the states of light and heavy holes and of the states of the spin-split-off band [8]. Such strains exist in QDs.

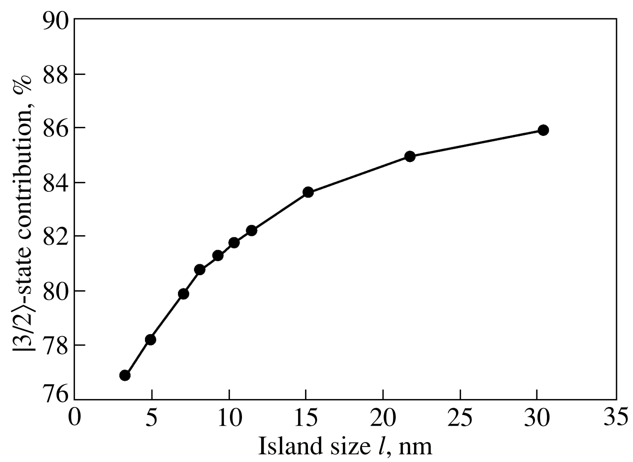

Fig. 3. Contribution from the $J_z = \pm 3/2$ states to the hole ground state as a function of the lateral size of a germanium island 1.5 nm in height.

Thus, for quantum dots, quantization in all three directions and nonhomogeneity of strains should significantly modify the *g* factor of hole states due to the mixing of the energy bands.

In [9], a method is suggested for calculating the *g* factor for hole states in quantum dots by using the tight-binding approach. This method takes into account a specific form of the quantizing potential (not necessarily described by an analytical function) and can be applied to calculate the *g* factor for QDs of any shape and of arbitrarily small size. This method can also be applied to electronic states in QDs.

If the Zeeman splitting of levels is small compared to the size-quantization energy, then the *g* factor depends only on the direction of the magnetic field and can be written in the first-order perturbation theory as

$$|g| = 2\sqrt{\langle\psi|\mathbf{n}\hat{\mathbf{M}}_{QD}|\psi\rangle^2 + \left|\langle\psi|\mathbf{n}\hat{\mathbf{M}}_{QD}|\psi^*\rangle\right|^2},$$

where **n** is a unit vector in the magnetic field direction, ψ and ψ^* are the wave functions of the level considered, and $\hat{\mathbf{M}}_{QD}$ is the magnetic-moment operator for a hole.

Calculations for a Ge/Si system with QDs show that the *g* factor of a hole in the ground state is strongly anisotropic, with the longitudinal component g_{zz} of the *g* factor being an order of magnitude larger than the transverse components g_{xx} and g_{yy}. For example, for a typical Ge island with base size $l = 15$ nm and height $h = 1.5$ nm, the values of the *g* factor components are $g_{zz} = 12.28$, $g_{xx} = 0.69$, and $g_{yy} = 1.59$.

From the calculated dependence of the *g* factor on the size of Ge islands, it follows that the *g*-factor anisotropy increases with the island size. Such a behavior of the *g* factor is mainly determined by the increased contribution from the states with the angular-momentum projections $J_z = \pm 3/2$ on the symmetry axis of the Ge island (Fig. 3).

The probability of Zeeman transitions is directly related to the character of the wave function. For the states with $J_z = \pm 3/2$ in the magnetic field $\mathbf{H} \parallel \mathbf{z}$, induced transitions between the Zeeman sublevels with $J_z = +3/2$ and $J_z = -3/2$ are forbidden by the selection rules; for allowed transitions, the condition $\Delta J_z = \pm 1$ must be satisfied. The admixture of the $J_z = \pm 1/2$ states facilitates the transitions between Zeeman sublevels of the ground state in the Ge island; therefore, with decreasing island size, the suppression of Zeeman transitions becomes weaker.

In the case of a dc magnetic field $\mathbf{H} \parallel \mathbf{z}$, the microwave field $\mathbf{H}_\omega$ lies in the plane of the QD layer and the Zeeman transition probability is proportional to the square of the matrix element of the magnetic moment component μ in the direction of the microwave field. In the special case of the microwave field $\mathbf{H}_\omega$ directed along [110], the particle magnetic moment component μ is proportional to the principal value g_{xx} of the **g** tensor and, for $\mathbf{H}_\omega \parallel [\bar{1}10]$, the particle-magnetic-moment component μ is proportional to g_{yy}. Accordingly, the transition probabilities are determined by the squares of these components of the *g* tensor, g_{xx}^2 ($\mathbf{H}_\omega \parallel [110]$) and g_{yy}^2 ($\mathbf{H}_\omega \parallel [\bar{1}10]$).

In the case of a dc magnetic field $\mathbf{H} \perp \mathbf{z}$, the magnetic-moment component μ lies in the plane perpendicular to the base plane and, in the special case of the microwave field $\mathbf{H}_\omega$ directed along [100], it is proportional to the principal value g_{zz} of the *g* tensor. The transition probability in this case is proportional to g_{zz}^2. For the obtained values of the *g* factor, the probabilities of induced transitions for the two directions of the magnetic field ($\mathbf{H} \parallel \mathbf{z}$ and $\mathbf{H} \perp \mathbf{z}$) differ by a factor of approximately 100.

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