Fine structure of the energy levels of an exciton bound on a boron atom in silicon

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The fine structure of the phononless emission line of an exciton bound on a boron atom in silicon, with and without compression along the (111) axis, is investigated. An interpretation is proposed for this structure that takes into account the valley-orbital splitting, *j–j* pairing of holes, and electron-hole exchange interaction.

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Impurity boron atoms in silicon create the smallest acceptor states with ionization energy equal to 45.7 meV, which agrees well with calculations in the effective mass approximation. We should therefore expect that the potential of the central cell occupied by the impurity ion should not be, in the case of boron, significantly manifested in the bound exciton, which, for this reason, could be a good model for investigating the

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structure of excitons bound by acceptors. The exciton bound by a group III acceptor in silicon contains two holes and an electron that moves in the field of the impurity ion. The splitting of the ground state of the bound exciton is due both to the interaction between light particles and valley-orbital splitting of the electron state. These splittings are relatively small in the case of boron, and it was not possible to resolve in Ref. 1 the structure of the corresponding emission line. In this work, this structure is investigated by an interference method,[2] with and without uniaxial compression of silicon, which permitted drawing some conclusions concerning the contribution of different types of interactions to the fine splitting of the energy levels of the bound exciton.

The spectra of the phononless emission line of the exciton bound on the boron atom are shown in Figs. 1 and 2. These spectra contain a large number of components. Under uniaxial compression, the fourfold-degenerate hole state Γ_8 splits into two states, which are degenerate only with respect to spin. For this reason, the two holes in the ground state form a spin singlet and cannot contribute to the splitting. Under compression in the (111) direction, equivalent with respect to the electronic valleys, the splitting of the ground state of the bound exciton could be caused only by valley-orbital splitting of electronic states. The spectrum on the right side of Fig. 1, recorded at a relatively high pressure P and low temperature, corresponds to predominant population of the ground state of the bound exciton under uniaxial compression. For this reason, the observed splitting $\cong 50$ μeV, which is due to valley-orbital splitting, determines its magnitude.

Valley-orbital splitting greatly complicates the spectra (Figs. 1 and 2). For this reason, we were able to follow the evolution of only some of the most intense compo-

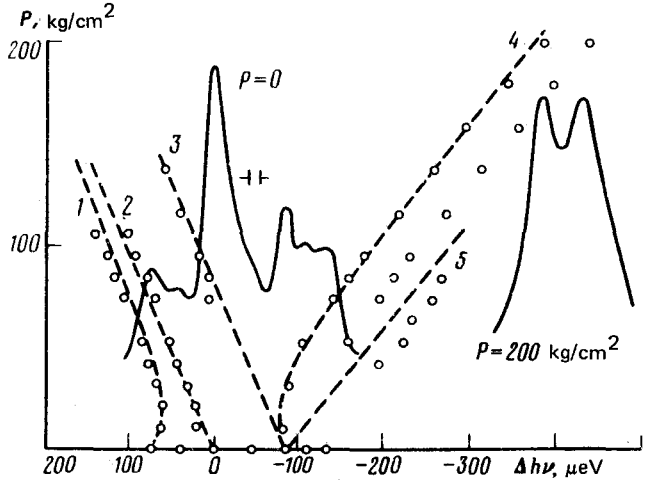

FIG. 1. Spectra of phononless emission line of excitons bound to boron atoms in silicon at pressures $P = 0$ (4.2 K) and $P = 200$ kg/cm^2 (2 K). The open circles show the experimental P dependence of the spectral position of components in the spectrum and the dashed curves represent the calculation. The boron concentration is 7×10^{15} cm^{-3}.

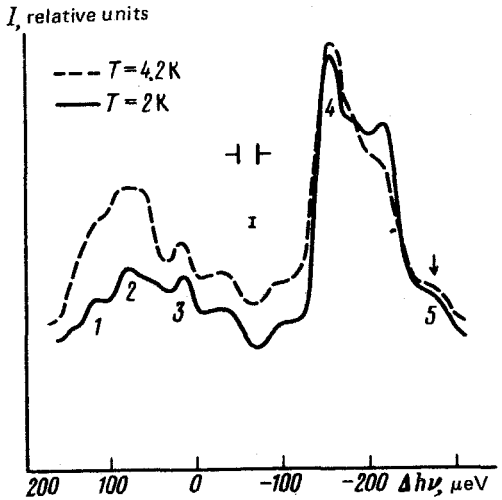

FIG. 2. Spectra of phononless emission lines of excitons bound to boron atoms at 2 and 4.2 K. $P = 85$ kg/cm^2.

nents with a variation in pressure P, which we associate with recombination of the electron from the state Γ_1. In contrast to the states Γ_3 and Γ_5, the electron wave function in the state Γ_1 does not have a node in the central cell, which increases the probability of a phononless radiative transition. For the same reason, we assume that the electron in the state Γ_1 has a higher energy than in the states Γ_3 and Γ_5, since it must be repelled more strongly by the negatively charged impurity ion. In addition, the electron in the symmetric state Γ_1 should not give rise to crystal-field splitting. We assume that in this case j–j pairing of holes and electron-hole exchange, which can be taken into account in the spherical approximation, give the main contribution to the splitting. The corresponding term in the Hamiltonian can be written in the form[3]

$$\mathcal{H} = A\mathbf{j}_1 \cdot \mathbf{j}_2 + B(\mathbf{j}_1 + \mathbf{j}_2) \cdot \mathbf{s}, \tag{1}$$

where $\mathbf{j}_1$, $\mathbf{j}_2$ are the angular momentum operators of the holes, $\mathbf{s}$ is the spin operator of the electron, and A and B are constants characterizing j–j pairing and electron-hole exchange. The eigenvalues are the energies E_1, E_3, E_5, which correspond to total angular momentum $J = 1/2$, $3/2$, and $5/2$ and which determine the spectral position of components in the absence of strain. Uniaxial compression along the (111) axis does not change the energy of the states with projections of the total angular momentum on the axis of compression $|M_J| = 5/2;3/2$. At the same time, strain leads to mixing and nonlinear variation of the ground-state energies with different J and identical projection of $|M_J| = 1/2$. This change is described by the equation[4]

$$(E_1 - E)(E_3 - E)(E_5 - E) = 4E_T^2\left[\frac{3}{5}(E_3 - E) + \frac{2}{5}(E_5 - E)\right], \tag{2}$$

where $2E_T$ is the strain-induced splitting of the hole state. The corresponding energy-level diagram and some optical transitions 1–5 are shown in Fig. 3. The dashed lines 1–5 in Fig. 1 show the spectral position of the components corresponding to these

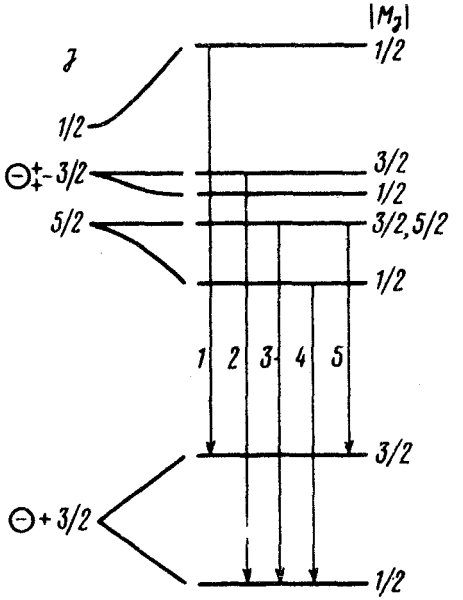

FIG. 3. Level diagram of an exciton bound to an acceptor with an electron in the state Γ_1 and a neutral acceptor with compression along the (111) axis. The arrows indicate identified optical transitions.

transitions as a function of pressure P calculated according to (2). The values of the energies E_1, E_3, E_5 are determined from the spectrum in Fig. 1 at $P = 0$, which gave $E_1 - E_3 = 74$ μeV and $E_3 - E_5 = 86$ μeV. Hence, the values of the interaction constants are $A = -21$ μeV and $B = -17$ μeV. The splittings of the hole state in the bound exciton and in the neutral acceptor were set equal to $2E_T$ (μeV) $= 2.96 \times P$ kg/cm^2, and the isotropic strain component was included by fitting an identical linear displacement of all levels as a function of pressure.

It is evident from Fig. 1 that components 3 and 5, whose spectral position depends linearly on P, evolve from the long-wavelength region of the spectrum with $P = 0$. This agrees with the choice of the state with $J = 5/2$ as the ground state, since the "linear" components cannot originate from the state with $J = 1/2$, while the intensity of the components with $J = 3/2$ at $P = 0$ must be maximum.[3] An analogous distribution of levels is characteristic for atoms. However, for excitons bound to aluminum and gallium atoms in silicon, the opposite distribution of terms is observed,[1] which is apparently a manifestation of the details of the potential of the central cell. It follows that boron is more of an "ideal" acceptor in silicon than other group III impurity atoms. We should also note the approximately equal contribution of hole j–j and electron-hole interactions (closeness of the values of the constants A and B) to the splitting of the states of the exciton bound on the boron atom. This confirms the large role of electron-hole exchange in multiparticle exciton-impurity complexes in silicon.[5]

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