Electron-electron exchange in many-valley semiconductors and the fine structure of many-exciton complexes in silicon

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The fine structure of the levels of an exciton bound by a neutral donor (ND) in silicon, which was detected recently in Ref. 1, is attributed to the exchange interaction between the electrons of different valleys and to the electron-hole exchange. The energies of the electron-electron (e-e) exchange and of the electron-hole (e-h) exchange are estimated.

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Kaminskiĭ, Karasyuk, and Pokrovskiĭ[1] have recently resolved the fine structure of the emission lines of bound, many-exciton complexes in silicon for the first time. Of particular interest is the detection of the fine structure of the line of an NDE_2 complex in silicon strained along the z[001] axis. The initial state of NDE_2 in a strained crystal is degenerate only with respect to the Γ_4 electron and is not split. Since the spins of the remaining two electrons, which fill the Γ_1 shell, as well as the spins of the two Γ_6 holes, are antiparallel, the *e-h* exchange must be missing. The splitting of the final state—the excited NDE_1^* state with two Γ_1 and Γ_4 electrons and a Γ_6 hole—is solely attributable to the exchange interaction. The experiments indicated above, therefore, made it possible for the first time to determine directly the exchange energies in silicon. Kaminskiĭ *et al.*[1] took into account only the exchange between the Γ_6 hole and the Γ_4 electron and assumed that the Γ_1 shell is a strongly localized orbital and hence that the Γ_1 electron does not interact with the hole. Although this model accounts for the observed splitting, the relation deduced from it for the line intensities is inconsistent with the experimental curve in Fig. 3 of Ref. 1, which has been reproduced in Fig. 1: According to this model, the spectrum consists of three lines, one of which is twice as intense as the other two. According to the the shell model,[2] the smooth wave function of the Γ_1 state is the same as that of the Γ_4 state, and these shells differ only in the fast functions: For the Γ_1 shell $U_{\Gamma_1} = 1/\sqrt{2}\,(U_1 + U_1)$ when the strain is large and for the Γ_4 shell $U_{\Gamma_4} = 1/\sqrt{2}\,(U_1 + U_1)$, where U_1 and U_1 are the Bloch electron functions of the [001] and [001] valleys, respectively. In terms of the shell model, therefore, the *e-h* exchange for Γ_1 and Γ_4 electrons must be the same; this exchange is determined by the expression

$$\mathcal{H}^{eh}_{ex} = \Delta_\perp (\mathbf{J}\mathbf{S}) + (\Delta_\parallel - \Delta_\perp)(J_z S_z) \cdot \qquad (1)$$

Here $\mathbf{J}$ is the moment of the hole ($\mathbf{J}_z = \pm 1/2$) and $\mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2$ is the total moment of the two electrons Γ_1 and Γ_2.

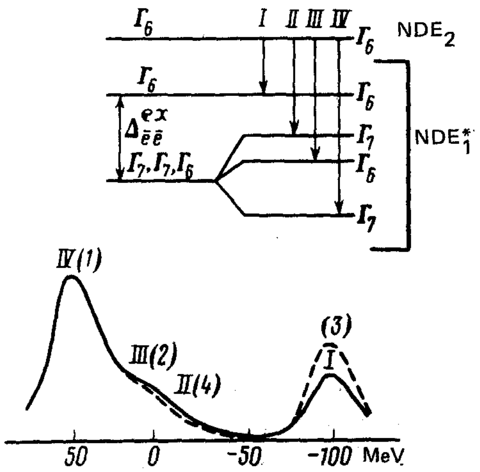

FIG. 1. Fine structure of the α_2 line in silicon compressed along [001]. The dashed line represents the experiment[1] and the solid line denotes the calculation from Table I for $\Delta_3 = 104\ \mu$eV, $\Delta_\perp = -47\ \mu$eV, $\Delta_{\parallel} = -12\ \mu$eV. The theoretical curve was broadened and combined with the experimental curve at the maximum of the line (1) IV.

According to Ref. 3, the *e-h* exchange in the unstrained crystal is described by the Hamiltonian,

$$\mathcal{H}^{eh}_{ex} = 2\Delta_1 (\mathbf{JS}) + 2\Delta_2 \sum_i J_i^3 S_i \,. \tag{2}$$

If the splitting of the hole levels due to strain is small compared with the binding energy of the hole, then the Δ_i constants in Eqs. (1) and (2) are connected by the relations: A contraction along the [001] axis gives $\Delta_\perp = 4\Delta_1 + 10\Delta_2$, $\Delta_\parallel = 2\Delta_1 + 1/2\,\Delta_2$; an expansion along the [001] gives $\Delta_\perp = 3\Delta_2$, $\Delta_\parallel = 6\Delta_1 + 27/2\,\Delta_2$.

In addition to the *e-h* exchange, we must take into account the *e-e* exchange between the electrons in different valleys. The closeness of the *g* factor of the electrons in silicon and $g_0 = 2$ and its isotropy indicate an absence of a noticeable mixing of the states of different zones as a result of spin-orbit interaction. The *e-e* exchange, therefore, is spherically isotropic, and is described by the Hamiltonian

$$\mathcal{H}^{ee}_{ex} = \Delta_3 (\mathbf{S}_1 \mathbf{S}_4) = \frac{1}{2}\Delta_3 (S^2 - 3/2) \,. \tag{3}$$

TABLE I.

№	Energy	Intensity	
		$I_\parallel$	$I_\perp$
I	Δ^{ex}_{ee}	2	1/2
II	$\Delta_\parallel (R-1)/4$	$3 - R^{-1}(1+8\xi)$	$\frac{1+R^{-1}}{4}$
III	$\Delta_\parallel/2$	0	1
IV	$-\Delta_\parallel (R+1)/4$	$3 + R^{-1}(1+8\xi)$	$\frac{1-R^{-1}}{4}$

$R = (1 + 8\xi^2)^{1/2} \quad \xi = \Delta_\perp/\Delta_\parallel$

The Δ_3 constant is described by the exchange interaction between the electrons of the [001] and [001] valleys

$$\Delta_3 = 2 J v^{-1} \int d^3 r_1 \, d^3 r_2 \, U_1^* (r_1) U_{\bar{1}} (r_1) \, V (|r_1 - r_2|) \, U_1 (r_2) U_{\bar{1}}^* (r_2), \tag{4}$$

where $J = \int |\phi(r,r,\ r_h)|^2 d^3 r d^3 r_h$, $\phi(r_1^e, r_2^e, r_h) = \phi(r_2^e, r_1^e, r_h)$ is a smooth NDE$_1$ function, and v is the volume.

Table I gives the energies of the four NDE$_1^*$ states with allowance for the *e-e* and *e-h* exchanges and for the abundance of transitions to these states, which were calculated using the selection rules[4] ; these selection rules for the NP transitions resulting from recombination of the Γ_1 electron coincide with the selection rules for the direct transitions at the Γ point. To determine the three constants $\Delta_\perp$, $\Delta_\parallel$, and Δ_3, we must know the location of the four lines, I–IV. The lines 1, 2, and 3, which are identified with the most intense (for $\Delta_\perp/\Delta_\parallel \geqslant 1$) lines IV, III, and I, respectively, in Table I, are indicated on the experimental curve in Ref. 1. If the weak peak (4) on the experimental curve belongs to the line II, then we find for the Δ_i constants $\Delta_3 = 104$ μeV, $\Delta_\perp = -47$ μeV, $\Delta_\parallel = -12$ μeV, consistent with $\Delta_1 = -48$ μeV, $\Delta_2 = -17$ μeV. The theoretical curve in Fig. 1, which was constructed for these values of Δ_i, differs from the experimental curve in that the intensity of the line (3) I is slightly lower. Note that these values of Δ_1 and Δ_2 are in agreement with the estimates of the exchange constant $|\Delta_{ex}^{eh}| \approx |\Delta_1| \approx 50$ μeV, which were determined in Ref. 5 from the spin relaxation time of the electron. A theoretical luminescence spectrum similar to the experimental spectrum could not be obtained in an unstrained crystal by taking into

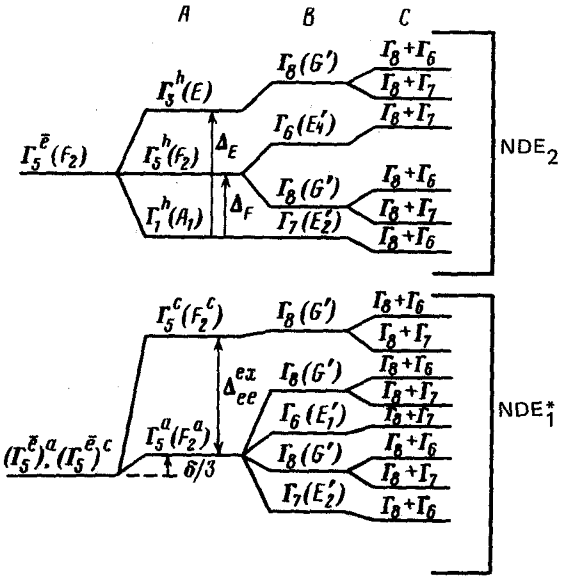

FIG. 2. Splitting of the $2\Gamma_1^e$, Γ_5^e, and $2\Gamma_8^h$ of NDE$_2$ and Γ_1^e, Γ_5^e, and Γ_8^h of NDE$_1^*$, with allowance for the *e-e* exchange, *e-h* exchange, exchange-valley splitting (A), *h-h* exchange (B) and for the crystal splitting (C) (the symbols of the representations in Ref. 7 are shown in the parentheses).

account the orbit-valley splitting, the *h-h* exchange (for NDE_2), the *e-h* exchange, and the *e-e* exchange (for NED_1^*). This presumably indicates the important role of crystal splitting—a similar situation to that in germanium.[6] The exchange-valley interaction[6] results only in the shift of all the $\Gamma_1\Gamma_5$ terms of the NDE_1^* state. The structure of the NDE_2 and NDE_1^* spectra is shown in Fig. 2, with allowance for these splittings. Since the exchange integrals (4) for the case in which the two electrons are in the "parallel" valleys (for example, [001] and [001]) differ slightly from the case in which they are in the "perpendicular" valleys ([001] and [010] or [100]), the *e-e* exchange for the $\Gamma_1\Gamma_5$ state may differ from that for the $\Gamma_1\Gamma_3$ state and from the exchange in a strained crystal Δ_3. For the same reason, the Δ_3 constant in Eq. (3) may depend on the strain, since the Γ_1 function arising from the mixing of the Γ_1 and Γ_3 states of an unstrained crystal changes with the strain.

Since all the transitions between the NDE_2-NDE_1^* states in Fig. 2 have been resolved, the spectrum must be comprised of a large number of lines. The experimental spectrum in Fig. 1 (Ref. 1) has 12 resolved lines, most of which correspond to several transitions in Fig. 2. We were therefore unable to select unambiguously the parameters of the NDE_2 and NDE_1^* spectra in an unstrained crystal from the data in this figure.

1. A. S. Kaminskiĭ, V. A. Karasyuk, and Ya. E. Pokrovskiĭ, Pis'ma Zh. Eksp. Teor. Riz. **33**, 141 (1981) [JETP Lett. **33**, 132 (1981)].
2. G. Kirczenow, Can. J. Phys. **55**, 1787 (1977).
3. G. E. Pikus and G. L. Bir, Zh. Eksp. Teor. Fiz. **60**, 195 (1971); **62**, 324 (1972) [Sov. Phys.—JETP **33**, 108 (1971); **35**, 174 (1972)].
4. G. E. Pikus, Fiz. Tverd. Tela **19**, 1653 (1977) [Sov. Phys. Solid State **19**, 965 (1977)].
5. P. D. Altukhov, K. N. El'tzov, G. E. Pikus, and A. A. Rogachev, Proc. 14th Intern. Conf. Phys. of Semicond., Edinburg, 1978, p. 379.
6. G. E. Pikus and N. S. Averkiev, Pis'ma Zh. Eksp. Teor. Fiz. **32**, 352 (1980) [JETP Lett. **32**, 328 (1980)].
7. L. D. Landau and E. M. Lifshitz, Kvantovaya mekhanika (Quantum Mechanics), Nauka, Moscow, 1974.

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