

Polarization of recombination radiation of bound multiexciton complexes (BMC) in silicon in a magnetic field

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We investigated the polarization of the *TO* emission lines of multiexciton complexes bound with boron. It was observed that the polarizations of the lines A^m with $m = 1, 2, 3$ excitons bound to the acceptor differ in magnitude and sign. This result confirms the BMC model, and cannot be explained by other existing models. A model of the BMC state is proposed, in which account is taken of the dependence of the energy on the type of valley states and on the orbit-valley splitting. The degree of polarization of the BMC emission lines calculated within the framework of this model agrees with the experimental results.

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As observed by Kaminskii and Pokrovskii,^[1] a series of narrow lines, which they attributed to recombination of pairs in BMC, appears in the emission spectra of silicon at high excitation levels. This interpretation was confirmed in^[2-5]. It was observed later that the character of the splitting of these lines under uniaxial deformation^[6-8] and in a transverse magnetic field^[7] is similar for all the lines of this series. On this basis, the authors of^[7,8] have concluded that these lines cannot be explained by means of the BMC model. Figure 1 shows the dependence of the degree of circular polarization of the *TO* emission lines of multi-exciton complexes bound with a neutral acceptor (*B*), on the magnetic field *H*. The measurements were made in a Faraday geometry at $H \parallel [111]$. The polarization was registered with the aid of the procedure described in^[10], the dependence of the degree of polarization on the magnetic field being plotted with an automatic *x-y* recorder. The radiation was excited with an argon laser whose beam was focused on the surface of the sample by a cylindrical lens. The polarization was measured at a spectral resolution ≈ 1.2 meV, while that of the emission spectra in the insert of Fig. 1 was measured with a resolution ≈ 0.5 meV. It is seen from Fig. 1 that the degree of polarization of the line A^2 exceeds the degree of polarization of the line A^1 , while the sign of the polarization of the line A^3 is reversed. Consequently, for the lines with $m = 1$ and 2, just as for the free exciton, the sign of the polarization is determined by the orientation of the holes, whereas the sign of the polarization of the $m = 3$ line is determined by the orientation of the electrons.^[10-12]

Thus, the experimental results obtained in the present study show that the spin states of the recombining electron and hole depends on *m*. This result can be explained by the BMC model proposed below, which is based on general symmetry considerations, but cannot be explained by means of the models proposed in^[7,8] and^[9].

It is natural to assume that the ground state of the BMC corresponds to smooth *S*-type functions for the electrons and holes (if the number of holes is $n_h \leq 4$), which are symmetrical with respect to permutation of spatial coordinates, while the spin functions of the holes are antisymmetrical and have a total angular momentum $j = 3/2, 0$ or $2/3, 0$ ^[13] at $n_h = 1, 2, 3$, and 4, respectively, as proposed in^[10-12] and^[14]. For two electrons in the BMC, the fast electron functions can be represented as the product of symmetrized valley functions and antisymmetrized spin functions or vice versa. As established in^[15], the binding energy of two electrons with a donor *D*⁻ in germanium

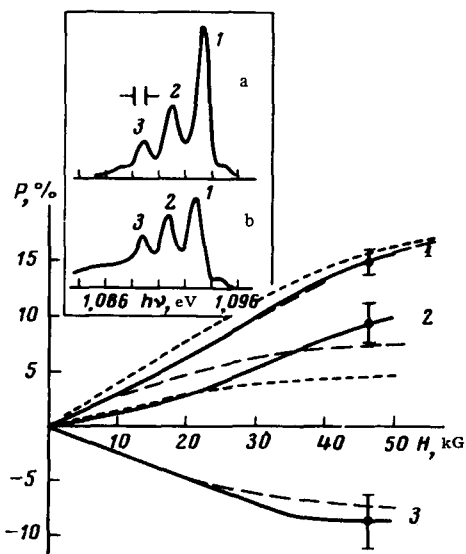


FIG. 1. Dependence of the degree of circular polarization P of the radiation on the magnetic field H at a temperature 1.9 K (Si : B, $n_A \approx 3 \times 10^{13} \text{ cm}^{-3}$). Solid curves—experiment. Dashed—theory at $\theta=2$, dotted—at $\theta=1$. The calculation was carried out at $\phi_{\text{TO}}=0.4$, $T=1.9$ K, $g_1=1.2$, $g_2=2$: 1— A^1 , $m=1$, $h\nu=1.0933$ eV; 2— A^2 , $m=2$, $h\nu=1.091$ eV; 3— A^3 , $m=3$, $h\nu=1.089$ eV. The vertical segments indicate the scatter of the experimental curves. Insert—BMC emission spectrum: a— $H=0$, b— $H=50$ kOe.

and silicon is maximal for states D_1^- in which both electrons are in different valleys, and is three times larger than the binding energy of the states D_0^- and D_1^- , in which electrons are in the same or in oppositely disposed valleys, owing to the decreased Coulomb repulsion of the electrons in the state D_1^- on account of the strong anisotropy of the electron effective mass. Therefore, for two-electron BMC in silicon, the lowest energy corresponds to states of the type xy (with the electrons in the valleys $x(100)$ and $y(010)$, whereas the states of the type xx and $x\bar{x}$ ($\bar{x}=\bar{1}00$) should have a higher energy. The short-range interaction (SI) with the impurity center leads to a splitting of the degenerate states, in analogy with the splitting produced in the states of neutral donors (ND) into A_1^+ , E^+ , and F_2^- . This splitting is determined by the corresponding Coulomb integrals between the Bloch functions of the valleys x , \bar{x} (J_1) and x , y (J_2). The equality of the energy of the terms E^+ and F_2^- for ND shows that $J_1=J_2=J$. (In this case $E_{A_1^+} - E_{E^+, F_2^-} = 6J$, $J < 0$). Table I lists the splittings of the SI states of the type sy , xx and $x\bar{x}$, with allowance for the mixing of the states xx and $x\bar{x}$ (at $J_1=J_2=J$). The SI also mixes the xy and xx , $x\bar{x}$ states underlined in Table I, which correspond to identical representations. The degree of this mixing depends on the splitting $\Delta = E_{xy}^0 - E_{xx}^0$ of the states in the effective mass approximation (SSEMA). In the right-hand column of Table I are indicated the states with allowance for mixing at $\Delta=0$, when the multielectron states can be regarded as the result of filling of the single-electron ND states, as suggested in^[16] (the mixed states are underlined). In light of^[15], we can regard the satisfaction of the conditions $|\Delta| \ll |J|$ as unlikely for BMC.

For three-electron states, when the SSEMA is taken into account, the lowest energy should be possessed by states of the type xyz with electrons in three mutually perpendicular valleys. States of the type $xx\bar{y}$ and $x\bar{x}y$ have a higher energy, while the states of the type $xx\bar{x}$ have the highest energy. The SI leads also to splitting of these states and to their partial mixing. Of all the xyz states, the lowest energy is possessed by the three states that are degenerate in spin only (all of equal energy), one of which corresponds to a total spin of electrons $S=3/2$ and to state A_2^+ antisymmetrical with respect to the valleys, while the two others correspond to a spin $X=1/2$. On the other hand, if there is no SSEMA, then, according to^[16], the minimum energy corresponds to states with $S=1/2$, in which both terms A_1^+ of the ND states and one of the levels E^+ or F_2^- are filled.

Starting from the foregoing model, we calculated the degree of circular polarization of the

TABLE I. Orbit-valley splitting of two-electron BMC states.

Energy in units of J	States of type				States in the absence of SSEMA	
	xy		$xx,$	$x\bar{x}$	$(\Delta = E_{xy}^o - E_{xx}^o = 0)$	
	symmetrical ($S = 0$)	antisymmetrical ($S = 1$)	symmetrical ($S = 0$)	antisymmetrical ($S = 1$)	symmetrical ($S = 0$)	antisymmetrical ($S = 1$)
-2	F_1^-, F_2^+	A_2^+, F_1^+, F_1^-	A_1^+, E^+	-	$F_2^- \times F_2^- = A_1^+ E^+, F_2^+$ $E^+ \times E^+ = A_1^+, E^+$ $E^+ \times F_2^- = F_1^-, F_2^-$	F_1^+ A_2^+ F_1^-, F_2^-
0	E^+	-	$F_2^-(xx)$	$F_2^-(x\bar{x})$	-	-
2	F_2^-	F_2^-	A_1^+, E^+	-	-	-
4	-	E^+	-	-	$A_1^+ \times F_2^- = F_2^-$ $A_1^+ \times E^+ = E^+$	F_2^- E^+
6	A_1^+	-	-	-	-	-
8	-	-	-	-	-	-
10	-	-	-	-	$A_1^+ \times A_1^+ = A_1^+$	-

radiation for the transitions $A^m - A^{m-1}$ at $m=1,2,3$, assuming that in the state A^1 we have $J=2$ and $S=1/2$, in the state A^2 we have $J=3/2, S=0$, while in the state A^3 we have $J=0$ and $S=1/2$. (Transitions from A^3 with $S=3/2$ are allowed only to A^2 at $S=1$.) Under these assumptions, the polarization of the $A^1 P_{TO}^1(H)$ line is determined by formulas (41) of^[12], and the respective polarizations of the lines A^2 and A^3 are

$$P_{TO}^2(H) = \frac{\theta \Phi_{TO} [3 \operatorname{sh}\left(\frac{3}{2} g_1 H^*\right) + \operatorname{sh}\left(\frac{1}{2} g_1 H^*\right)]}{[2(4 + \theta) - \Phi_{TO}(4 - \theta)] \operatorname{ch}\left(\frac{3}{2} g_1 H^*\right) + [2(4 + \theta) + \Phi_{TO}(4 - \theta)] \operatorname{ch}\left(\frac{1}{2} g_1 H^*\right)} \quad (1)$$

$$P_{TO}^3(H) = -\frac{1}{2} \Phi_{TO} \operatorname{th}\left(\frac{1}{2} g_1 H^*\right). \quad (2)$$

Here, as in^[12], g_1 and g are the g -factors of the holes and electrons, $H^* = \mu_0 H / kT$, $\Phi_{TO} = 0.4$.^[10] $\theta = 1$, if only transitions to the state A^1 with $J=2$ contribute to the radiation, and $\theta = 2$ if the transitions go both to the state with $J=2$ and to the state with $J=0$.

The theoretical plots of (1) and (2) are shown in Fig. 1 by dashed and dotted lines. The depolarization factor is determined from the degree of polarization of the line A^1 .^[10] It is seen from Fig. 1 that the theoretical curve agrees with the experimental ones within the limits of the scatter indicated in Fig. 1; this scatter is connected principally with the inaccuracy of the setting of the spectral position of the monochromator slit to the maximum of the emission line, and to the small overlap of the A^m lines.

It was suggested in^[16,17] that the customarily observed lines (a^m) correspond to transitions to $n-1$ excited states, while transitions to $m-1$ ground states correspond to the lines β^{m-1} observed in^[17]. In accordance with the general BMC scheme proposed in the present paper, transitions to the excited states should correspond to series of lines. In the case of transitions in which phonons take part, the polarization should be the same for all the lines corresponding to a definite final state $n-1$, whereas for phononless transitions it should depend on the type of state $m-1$. Simultaneous measurements of the polarization of the phonon and phononless series make it possible to establish the transition scheme corresponding to the observed lines.

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