Fine structure in the spectrum of the recombination radiation of excitons bound to acceptors in silicon

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(Submitted 26 December 1991; resubmitted 15 January 1992)
Pis'ma Zh. Eksp. Teor. Fiz. **55**, No. 4, 245–247 (25 February 1992)

For bound excitons, the fine-structure splitting of the spectral components which stem from the valley-orbital interaction can be explained on the basis that the symmetry of an acceptor center is lowered by the Jahn–Teller effect.

We have previously studied[1] the recombination-radiation spectrum of excitons bound at acceptors (group III elements) in single-crystal silicon. The structure observed in the recombination-radiation spectrum was explained on the basis of a valley-orbit splitting of the ground state of bound excitons. Thewalt and Brake[2] showed that each of the lines which we observed was split in two. On the other hand, they were unable to explain this additional splitting.[2] In the present letter we report some additional experimental data, and we offer an explanation for this splitting.

We restricted the experiments to silicon single crystals doped with aluminum and gallium. The samples were immersed in λ-helium and excited by the beam from an LGN-40-A argon laser. The light emitted as a result by excitons bound at acceptors was analyzed by a spectrometer including a Fabry–Perot interferometer and detected by a cooled photomultiplier.[3] The final step of the processing was to deconvolve the spectrum. This step partially eliminated the distortions introduced by the spectrometer.[1)] The resulting spectral resolution was 5 μeV. The uniaxial-compression method used to produce a uniform strain in the samples is described in Ref. 3.

Figure 1 shows some typical spectra of the recombination radiation of excitons bound to dopant aluminum atoms in silicon. The spectrum in Fig. 1a is the experimental spectrum of the recombination radiation of bound excitons. Figure 1b shows the spectrum of this light after a mathematical processing. This spectrum agrees well with that found in Ref. 2. Figure 1c shows a spectrum found under conditions of uniaxial compression of a sample along the [111] direction. Figure 2 shows similar spectra of the recombination radiation of excitons bound to dopant gallium atoms.

The recombination-radiation spectra measured in the absence of a uniaxial compression of the samples (Figs. 1b and 2b) are characterized by a splitting of each line into at least two components. We attribute[1] this splitting to a valley–orbital splitting of the ground state of a bound exciton. In the case of gallium (Fig. 2b) this splitting is not as obvious as in the case of aluminum. When the samples are compressed along the [111] direction, the spectrum of the recombination radiation changes sharply: The final acceptor state, Γ_8 (after the optical transition), splits into two states, Γ_4 and $\Gamma_6+\Gamma_7$. Two identical groups of lines appear in the spectra. Each of these groups corresponds to optical transitions to these states.[1] We recall that a deformation of silicon along the [111] direction does not lift the electron degeneracy with respect to

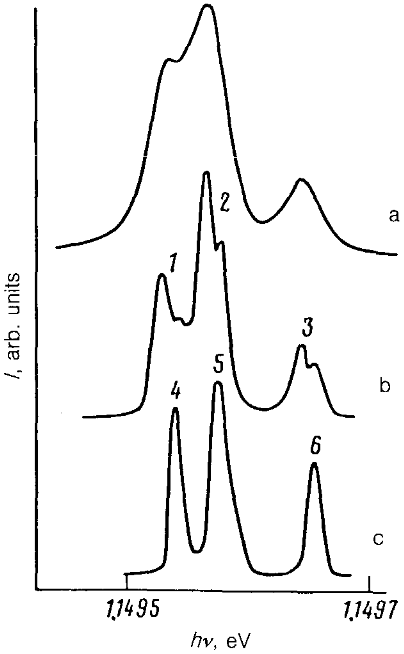

FIG. 1. Spectrum of the α-NP components of the emission by excitons bound at dopant aluminum atoms in silicon ($N_{\rm Al} = 2\times10^{14}$ cm^{-3}) at 2K. a—$P = 0$, experimental spectrum; b—$P = 0$, spectrum found after elimination of the distortions introduced by the spectrometer; c—$P \parallel [111]$, $P = 17$ MPa, after removal of the distortions introduced by the spectrometer. The numerals specify the spectral components in the notation of Ref. 1.

valleys, and it should not have any substantial effect on the valley–orbital interaction of an electron with the central cell. It is thus natural that the spectra corresponding to these transitions would be the same (aside from the finer structure) as the spectra found at $P = 0$, where P is the pressure. Figures 1c and 2c show only fragments of the recombination-radiation spectra corresponding to transitions to the $\Gamma_6 + \Gamma_7$ state. An important point is that the fine structure disappears when the samples are compressed along the [111] direction, and the emission lines become narrower by a factor of about two. It also follows that the fine splitting of the recombination-radiation lines cannot be explained in terms of a valley–orbital interaction.

We believe that the fine-structure splitting of the recombination-radiation lines of excitons bound at acceptors (at $P = 0$) results from a lowering of the symmetry of the acceptor because of a static or dynamic Jahn–Teller effect.

In the case of the static Jahn–Teller effect, an acceptor is displaced from its lattice site as the result of an interaction with a local vibrational mode. It moves to one of the potential wells corresponding to a minimum of the potential energy of the acceptor center and of the exciton bound to it. In the adiabatic approximation, the quadruply degenerate final state of the acceptor, Γ_8, should split into two doubly degenerate states. According to the Franck–Condon principle, this splitting should lead to a

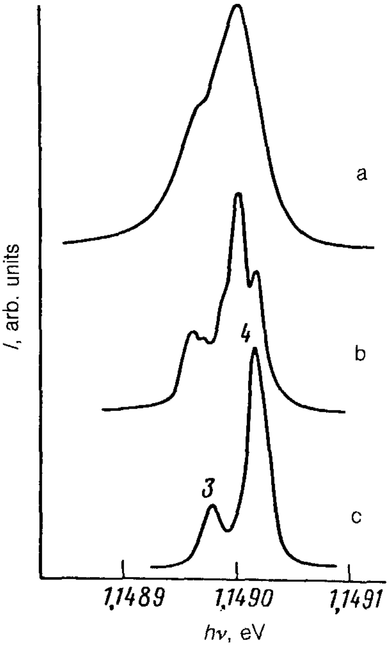

FIG. 2. Spectrum of the α-*NP* components of the emission by excitons bound at dopant gallium atoms in silicon ($N_{\mathrm{Ga}}=7\times10^{14}$ cm^{-3}) at 2 K. a—$P=0$, experimental spectrum; b—$P=0$, spectrum obtained after removal of the distortions introduced by the spectrometer;[4] c—$P\parallel[111]$, $P=8$ MPa, after removal of the distortions introduced by the spectrometer. The numerals have the same meaning as in Fig. 1.

splitting of the lines in the recombination-radiation spectra. When the crystal is subjected to uniaxial compression, the degeneracy of the ground state of the acceptor is lifted. For this reason, there is no fine structure in the recombination-radiation spectra of the uniaxially compressed crystals.

In the case of the dynamic Jahn–Teller effect, there may be a resonant tunneling of a dopant atom between equivalent potential wells. The degeneracy of the levels of the acceptor center is lifted in the process, and the recombination-radiation lines split as a result. A uniaxial compression of a crystal should suppress this tunneling and thus the associated level splitting.

Since the nature of the interaction between the holes bound at an acceptor with various vibrational modes is not known, it is difficult to say whether the static or dynamic Jahn–Teller effect is operating in this case.

As the symmetry of an acceptor center is lowered as the result of a displacement of an atom from a lattice site, the electron terms Γ_3 and Γ_5 should split, and lines 1 and 2 (Fig. 1b), which correspond to these terms, should have a structure more complex than that of line 3 (Fig. 1). The latter line corresponds to the electron term Γ_1. What we observe, in contrast, is roughly the same splitting for all three lines. The most likely explanation for the absence of an additional splitting of lines 1 and 2 is that the interaction of (on the one hand) a greatly delocalized electron, whose wave function vanishes at the center, with (on the other) the local vibrations of the atomic center is considerably weaker than the phonon–hole interaction which causes the Jahn–Teller effect.

For donor centers, we do not observe a corresponding splitting of the lines in the recombination-radiation spectra. This situation is natural, since the electronic ground state of a donor is not degenerate, and the Jahn–Teller effect cannot cause a splitting of the spectral lines of the recombination radiation.

We wish to thank E. L. Kosarev and E. R. Podolyak (IFP, Russian Academy of Sciences) for furnishing the spectrum-processing program and for consultations regarding its use, which made this study possible. We also thank N. S. Averkiev and A. A. Gutkin (Leningrad Physicotechnical Institute, Russian Academy of Sciences) for a productive discussion of these results.

1) The program[4] which we used makes it possible to achieve a limiting ultraresolution at a given signal-to-noise ratio. This program increases the spectral resolution by a factor of several units, and (a particularly important point) it does not introduce false lines, in contrast with other programs of this type.

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Translated by D. Parsons