Intensity of extrinsic optical transitions in phosphorus-doped silicon

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(Submitted 28 November 1988)
Pis'ma Zh. Eksp. Teor. Fiz. **49**, No. 1, 39–42 (10 January 1989)

The oscillator strengths f_{nP_M} of extrinsic optical transitions in silicon doped with phosphorus to a concentration $N_P = 1.7 \times 10^{14}$ cm^{-3} have been determined. The values found for f_{nP_M} are approximately half those predicted by the theory of Beĭnikhes and Kogan {Zh. Eksp. Teor. Fix. **93**, 285 (1987) [Sov. Phys. JETP **66**, 164 (1987)]}.

The optical absorption spectra of slight impurities in multivalley semiconductors have been used for the most part to study the structure of the impurity energy levels, transition energies, and the shapes and widths of lines (see, for example, the review by Ramdas and Rodriguez[1]). Very little information has been published on the photoionization cross sections[2,3] and, especially, on the oscillator strengths of intraimpurity optical transitions for slight impurities in silicon and germanium. The oscillator strengths have recently been determined[4] for the two brightest transitions in group V donors and III acceptors in germanium. Bambakidis and Brown[5] have reported the areas under the spectral lines of gallium and indium in silicon, found from unpublished data. The corresponding oscillator strengths can be found from these areas (but these strengths were not reported in Ref. 5). In the present letter we report measurements of the oscillator strengths of transitions in Si:P.

The data reported here refer to a sample cut from a float-zoned phosphorus-doped silicon crystal. The phosphorus concentration was found from measurements of the Hall coefficient at room temperature to be $N_P = 1.7 \times 10^{14}$ cm^{-3}. The degree of

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compensation of the major impurity was found from the bound-exciton luminescence spectra to be 0.03. All the measurements were carried out on a Bruker 113v Fourier spectrometer. In some of the experiments we used a filter of black polyethylene (in addition to the regular filters) in order to eliminate the slight interband illumination. It was found that for our samples this polyethylene filter causes no significant change in the results of the measurements. Transmission spectra measured at $T = 4.4$ K were normalized to the signal level in the gap between the lines in the long-wavelength part of the same spectrum (far from the continuum).

Figure 1 shows an extrinsic absorption spectrum recorded at a spectrometer resolution of 0.1 cm^{-1}. Analysis of the lines, shown in greatly enlarged scale along the frequency axis, revealed that their shape was something between Lorentzian and Gaussian. The total width at half-maximum ranged from 0.34 to 0.45 cm^{-1} for the various lines. In calculating the absorption we allowed for multiple reflection of light in the sample; the area under each line was found by an integration over its contour. Using the sum rule,[6,7] we find the following expression for the oscillator strength of the optical transition from the $1s(A_1)$ ground state (at a low temperature, and in the absence of intense background light, only this state is occupied) to the nP_M state (the

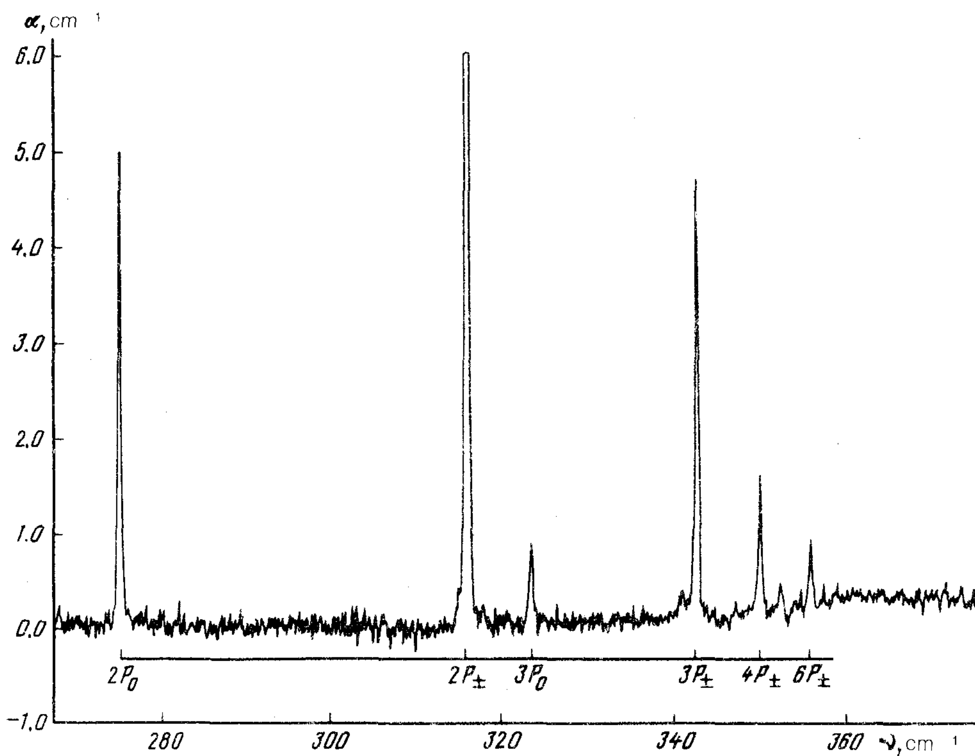

FIG. 1. Extrinsic absorption spectrum in Si:P. The most intense lines are identified. Strong absorption is observed at the center of the $1s(A_1) \to 2P$ line (this line has been clipped in this figure).

TABLE I.

Transition		ν_0, cm^{-1}	$(S_L/N_P)\times 10^{14}$ cm	$(f_{n,P_M})\times 10^3$ Experimental	Theoretical	f_{nP_M} (expt) / f_{nP_M} (theo)
$1s(A_1) \rightarrow$	$2P_0$	275.13	1.64	16.24	31.3	0.52
	$2P_\pm$	316.02	$\gtrsim 7.08$	$\gtrsim 70$	133	$\gtrsim 0.52$
	$3P_0$	323.46			6.44	
	$3P_\pm$	342.45	1.6	15.8	30.4	0.52
	$4P_\pm$	349.95	0.58	5.7	10.8	0.53
	$5P_\pm$	352.31	0.13	1.3	3.7	0.35
	$7P_0$	354.32	0.03	0.29	0.74	0.4
	$6P_\pm$	355.81	0.36	3.56	9.09	0.39
	$8P_\pm$	358.83	0.15	1.5	4.3	0.35

notation is explained in Ref. 7):

$$f_{nP_M} = \frac{n\bar{m}c^2}{\pi e^2}\left(\frac{E_0}{E_{eff}}\right)^2 \frac{S_L}{N_P} = 0.987\times 10^{12}\,\mathrm{cm}^{-1}\frac{S_L}{N_P}, \qquad S_L = \int_L \alpha d\nu .$$

Here $n = 3.387$ is the refractive index of the crystal[8]; $\bar{m} = 3/(1/m_l + 2/m_t) = 0.258m_0$ is the average effective mass of the charge carriers; α and ν are the absorption coefficient and emission frequency, expressed in units of reciprocal centimeters; and $E_0/E_{\rm eff}$ is the ratio of the average field to the effective field which induces the transition. For slight impurities in silicon and germanium we would have[9] $E_0/E_{\rm eff} = 1$. Table I shows the line positions (ν_0), the measured areas under the lines, divided by the impurity concentration; the oscillator strengths calculated from them; and their theoretical values for a phosphorus impurity in silicon.[7] It can be seen from this table that the oscillator strengths found by the method outlined above are smaller by a factor of two, and by nearly a factor of three for shallow final states, than predicted by the theory. Interestingly, oscillator strengths roughly half those predicted by the theory were also found by Rotsaert *et al.*[4] for intense transitions for impurities (Sb, P, and As) in germanium.

For donors in silicon, there has apparently been no previous determination of the oscillator strengths, so in order to compare our results with data which could be found from published extrinsic absorption spectra we made use of Ref. 10, which shows, in an acceptable scale, lines of phosphorus in transmutation-doped silicon ($2P_0$, $2P_\pm$, and $3P_\pm$), along with the impurity concentrations. The calculated oscillator strengths for these lines are $f_{2P_0} = 14.1\times 10^{-3}$, $f_{2P_\pm} = 84\times 10^{-3}$, $f_{3P_\pm} = 16\times 10^{-3}$.

In summary, an analysis of the spectra which have been reported in the literature

yields oscillator strengths close to those which we have found, confirming the roughly twofold discrepancy with the theory of Ref. 7 which we have observed in silicon and which has been observed elsewhere[4] in germanium. On the other hand, Beĭnikhes and Kogan[7] report some convincing evidence for the validity of the oscillator-strength calculations, in particular, an agreement of the polarizabilities found from these strengths with experimental data (see Ref. 11 regarding P in Si). At present, we can explain only why the decrease in the oscillator strengths for shallow final states in comparison with the theory is greater than for other transitions. This decrease results from a transition of some of the absorption into the continuum (the pedestal of the lines), which increases smoothly toward the ionization energy and which is observed both in our and other spectra (Ref. 12, for example). This continuum arises from an overlap of high-lying final states of transitions in close-lying impurity centers. The difference between the experimental and theoretical oscillator strengths might be explained on the basis that the effective field at the impurity is slightly weaker (by a factor of 1.5) than the average field in the crystal. At the moment, however, we have no grounds for making such a suggestion.

We wish to thank A. S. Kaminskiĭ and A. N. Safonov for furnishing the crystal and for measuring the degree of impurity compensation in it, Yu. A. Nechneev for determining the phosphorus concentration in the sample, and Sh. M. Kogan and I. L. Beĭnikhes for a discussion of these results.

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Translated by Dave Parsons