Interaction of charge carriers in multiparticle exciton-impurity complexes in silicon

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It is shown that the "natural" width of bound-exciton emission lines in phosphorus-doped silicon does not exceed 5 μeV and that the emission lines of multiparticle complexes have a large number of components whose splitting is explained by the interaction between the holes and between the holes and the outer electrons.

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We have used the interference method[1] to investigate the shape and fine structure of the phononless emission lines α_m of the multiparticle exciton-impurity complexes P_m bound by phosphorus atoms in silicon (m is the number of electron-hole pairs). The fine structure appears as a result of interaction of charge carriers in the complexes, which splits the initial P_m state and the final P_{m-1} state.[2,3] The α_1 line does not have a

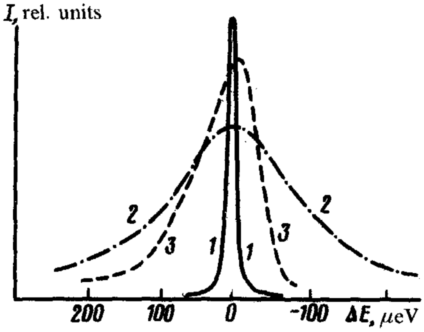

FIG. 1. Phononless emission lines of excitons bound to phosphorus atoms (concentration $P_0 = 2\times 10^{14}$ cm^{-3}) in silicon at 4.2 K. Neutron-doped sample SV – 1: 1, α_1 line; 2, α_1^{2S} line. Sample with phosphorus concentration of 7×10^{17} cm^{-3} grown in a quartz crucible: 3, α_1 line.

fine structure, since the two electrons, which form the singlet Γ_1 (ee), cannot split the hole level Γ_8 in the initial state $P_1\{\Gamma_8(h)\Gamma_1(ee)\}$, while the final state $P_0\{\Gamma_1(e)\}$ has only one electron. Therefore, an analysis of the shape of the α_1 line makes it possible to draw conclusions about the broadening and splitting of the emission lines of complexes, which are not related to charge-carrier interaction. We can see in Fig. 1 that the narrowest α_1 line is observed in silicon crystals grown by the crucibleless zone crystallization method and doped with phosphorus by means of neutron irradiation. The width of the α_1 line, with allowance for the finite resolution, does not exceed 5 μeV. In the decay of P_1 with the production of a donor in the excited $2S$ state the α_1^{2S} line is broadened considerably compared with α_1, because of the small lifetime $\sim 5\times 10^{12}$ sec) of the excited state. A strong inhomogeneous broadening of the α_1 line was observed in crystals grown from quartz crucibles and therefore containing an appreciable ($\sim 10^{18}$ cm^{-3}) concentration of oxygen. The imperfect crystals investigated in Ref. 3 apparently caused a broadening of the α_1 line to 50 μeV, an unsatisfactory resolution of the structure of the α_2 line and an erroneous interpretation of the results.

It can be seen in Fig. 2 that the α_2 emission line consists of a large number of components whose splitting is due to the interaction of charge carriers in the initial state P_2 $\{\Gamma_8(hh)\Gamma_1(ee)\Gamma_{35}(e)\}$ and the final state P_1 $\{\Gamma_8(h)\Gamma_1(e)\Gamma_{35}(e)\}$. The main feature of this splitting can be explained by taking into account only the interaction between the holes and the exchange interaction of holes with an electron of the outer Γ_5 shell. Interaction with electrons in the Γ_1 shell can be ignored, since this shell in P_2 is filled, and the electron in P_1, which remains in a highly localized orbital, does not interact strongly with the rest of the charge carriers. The Γ_3 electron shell at 2K must be slightly populated, since it lies in P_1 above the Γ_5 shell by approximately[4] 600 μeV. Since the anisotropy of the effective electron mass in silicon is not very large and since the crystal splitting $\Gamma_8(h)\times\Gamma_5(e)$ must be slight, we shall assume that the wave function of the electron in the Γ_5 shell is transformed as a Γ_6 spinor. In these approximations the initial state in the P_2 complex must split into four levels $\{\Gamma_8(h)\times\Gamma_8(h)\}\times\Gamma_6(e) = \Gamma_6 + \Gamma_7 + \Gamma_8 + \Gamma_8$. The final P_1 state is split into three levels $\Gamma_8(h)\times\Gamma_6(e) = \Gamma_3 + \Gamma_4 + \Gamma_5$. The splitting scheme for the structure of the α_2 line is shown in Fig. 2. To compare the experimental spectrum with the diagram, we have

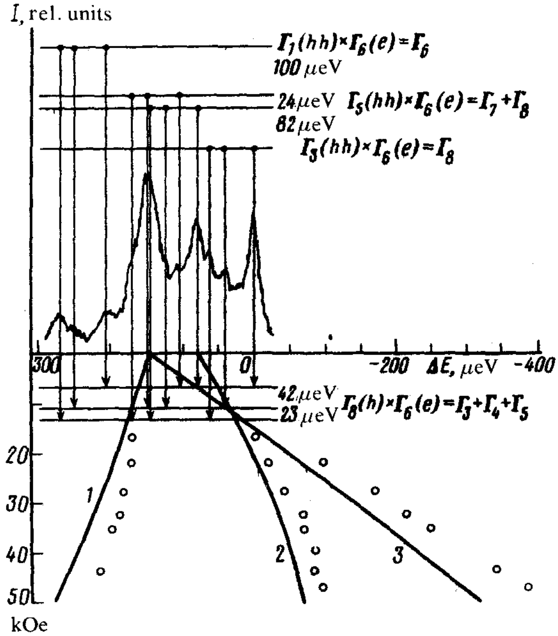

FIG. 2. Fine structure of the α_2 line of sample SV – 1 at 2K and $H = 0$. The arrows depicting the transitions from the initial P_2 state to the final P_1 state indicate the predicted location of the emission lines along the horizontal energy axis, in accordance with the splitting of the P_2 and P_1 levels in the diagram. The Zeeman components of the α_2 line (circles) are plotted in the lower part of the figure as a function of the intensity of the magnetic field H||(111). The dependence of the shift of the Zeeman components of the α_1 line on H (solid curves) for the analogous electron transitions is also shown there.

matched the arrow corresponding to the radiative transition with minimum energy on the horizontal energy scale with the location of the longest wavelength component of the spectrum and the location of the remaining arrows illustrating the transitions is determined by the splitting of the initial and final states indicated in the diagram. We can see in Fig. 2 that this scheme describes well the structure of the α_2 line

The Zeeman spectrum of α_2 in a magnetic field $H \geqslant 20$ kOe consists of three main components[5]

$$P_2\left\{\Gamma_8\left(-\frac{3}{2},-\frac{1}{2}\right)\Gamma_1\left(+\frac{1}{2},-\frac{1}{2}\right)\Gamma_5\left(-\frac{1}{2}\right)\right\}\to P_1\left\{\begin{array}{r}\left\{\Gamma_8\left(-\frac{3}{2}\right)\Gamma_1\left(-\frac{1}{2}\right)\Gamma_5\left(-\frac{1}{2}\right)\right\}\\ (1)\\ \left\{\Gamma_8\left(-\frac{1}{2}\right)\Gamma_1\left(-\frac{1}{2}\right)\Gamma_5\left(-\frac{1}{2}\right)\right\}\\ (2)\\ \left\{\Gamma_8\left(-\frac{3}{2}\right)\Gamma_1\left(+\frac{1}{2}\right)\Gamma_5\left(-\frac{1}{2}\right)\right\}\\ (3)\end{array}\right.$$

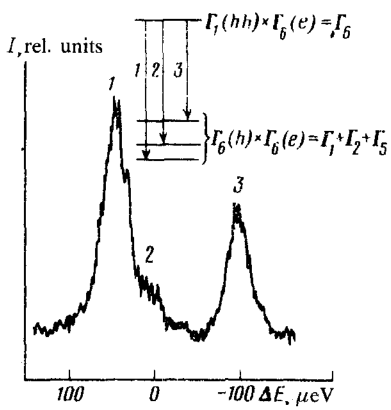

FIG. 3. Fine structure of the α_2 line at 2K produced as a result of compression (390 kgf/cm^2) of the SV – 1 sample in the (001) direction.

whose location is plotted in Fig. 2 as a function of H. The dependence on H of the shift of the Zeeman components of the α_1 line for the corresponding electron transitions is represented by the solid lines in Fig. 2. We can see in Fig. 2 that the dependence of the shift of the Zeeman components of the α_2 line is close to that for the analogous components of the α_1 line. Used in the identification of the transitions, this fact made it possible to reliably identify the spectral regions of the α_2 line from which the corresponding Zeeman components originate. We can see that the components 1 and 3 of the α_2 line originate from the same spectral region at $H = 0$, and the component 2 arises from another region of the original spectrum. It follows from this that the interaction between a hole and an electron of the outer Γ_5 shell gives the major contribution to the splitting of the final state P_1, while the interaction with the electron of the Γ_1 shell does not result in noticeable splitting.

When the silicon is compressed in the (001) direction, the symmetry is reduced to D_{2d} and the lowest energy state of the holes is Γ_6 with the moment $\frac{1}{2}$, which is degenerated only in spin. The electron state Γ_1 is not split, while the Γ_{35} state is split into several branches, the lowest of which corresponds to the nondegenerate Γ_4 state. Thus, the ground state P_2 is not split with uniaxial compression. The final state P_1 is split into three states $\Gamma_6(h)\times\Gamma_6(e) = \Gamma_1 + \Gamma_2 + \Gamma_3$, because of the exchange interaction of a hole with an electron from the outer Γ_4 shell. The spectrum of the α_2 line for uniaxial compression along (001) is shown in Fig. 3, together with the transition scheme. We note that the α_2 line is also a triplet as a result of stretching along the (001) axis; this comfirms the validity of there approximations.

Thus, the proposed model makes it possible to explain the fine structure of the α_2 line and its splitting in magnetic and strain fields.

The asymmetric spectra of the α_3 and α_4 lines have a large number of anomalies, which indicates that they consist of many components. However, the individual components could not be resolved, probably because of their noticeable broadening, since the P_{m-1} complexes are produced in the excited state as a result of emission of the

α_m line. In this case the time of relaxation of one of the $m-1$ electrons of the Γ_{35} shell to a partially filled Γ_1 shell must decrease as m increases.

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