Influence of band degeneracy on the formation of multiparticle exciton-impurity complexes (E_mIC)

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We investigated the influence of uniaxial deformation on the recombination radiation (RR) spectra of E_mIC in Si(P) and Si(B). It is shown that the band degeneracy is a necessary condition for the formation of E_mIC.

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The RR spectra of doped silicon at high excitation levels contain a series of narrow lines, first observed in[1] and attributed there to recombination of excitons into E_mIC. This interpretation was further developed in[2–5]. Investigating the character of the RR line splitting of E_mIC under uniaxial deformation, the authors of[6] have reached the conclusion that the band splitting does not influence the formation of the E_mIC. Later, however, on the basis of a study of the splitting of these lines under uniaxial deformations and in a magnetic field, the E_mIC model was totally rejected in[7,8].

We have investigated in detail the influence of uniaxial deformation on the RR spectra of E_mIC in Si(P)($N_P=2\cdot10^{14}$ cm^{-3}) and in Si(B)($N_B=3\cdot10^{12}$ ti $5\cdot10^{13}$ cm^{-3}). The uniaxial deformation was produced by the procedure described in [9]. The optical excitation was with a 100-mW GaAs laser, the spectral instrument was a double monochromator with dispersion 10 Å/mm in the working region, and the RR receiver was a cooled FÉU-62 photomultiplier operating in the photon-counting regime. In the undeformed silicon, both bands are degenerate. Elastic deformation along [111] splits the valence band into two bands that are doubly degenerate in spin only, while the conduction band remains unchanged (6 valleys). In this case at $T=1.8$ K the RR lines of the E_mIC that contain one or two holes (i.e., with $m=1(BE)$ for Si(B) and with $m=1(\alpha_1)$ and $2(\alpha_2)$ for Si(P) are split (Fig. 1) and are observed in the spectrum at all the investigated deformations ($P<70$ kgf/mm^2). The RR lines of E_mIC with three and four holes [BE_2 and BE_3 for Si(B) and α_3 and α_4 for Si(P)] are split at small deformations into doublets, and vanish completely from the spectrum at $P>10$ kgf/mm^2. The splitting of these lines is close to the splitting Δ_v of the valence band.

These experimental results agree well with the shell model of the E_mIC,[3] according to which the electrons and holes fill the shells in accordance with the Pauli principle, with allowance for the symmetry of the impurity centers. Figure 2 shows the schemes, expected on the basis of this model, of the transitions in E_mIC for Si(P) and Si(B), both undeformed and deformed along [111]. At 1.8 K and $\Delta_v>0.2$ meV it is necessary to consider only transitions from the ground states. The splitting picture is then in full agreement with the experimentally observed one. We note that transitions from (1/2, −1/2) into ($\pm$3/2) and from [1/2, −1/2, $\pm$3/2) into (3/2, −3/2) are

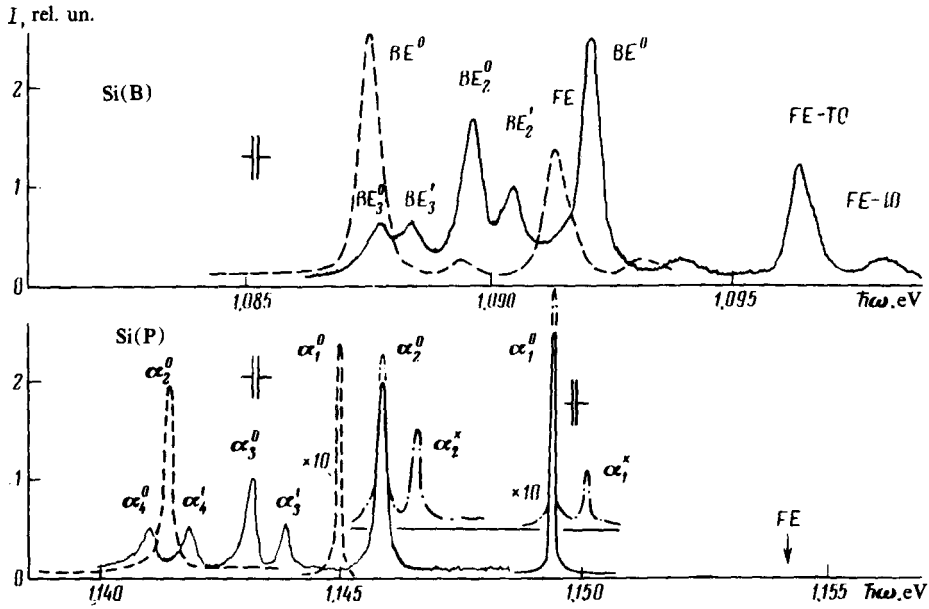

FIG. 1. RR spectra of E_mIC in silicon deformed along [111]. $T=1.8$ K, solid lines–$P=2$ kgf/mm², dashed–$P=6$ kgf/mm²; dash-dot–$T=7$ K, $P=2$ kgf/mm².

forbidden. The intensity ratio of the lines in the doublets ($\approx 1/2$ or ≈ 1) reflects the ratio of the statistical weights for the holes ($\pm 1/2$) and ($\pm 3/2$) in the initial complex. At higher temperatures, the doublet structure is observed also for the lines α_1 and α_2. This agrees with[8] and reflects the presence of thermodynamic-equilibrium complexes that include the holes ($\pm 3/2$). However, in contrast to the authors of[8], we call attention to the fact that the ratio $\exp(\Delta/kT)$ for the line intensities in the doublet is valid only for α_1; it is close to $(1+(1/4)e^{\Delta/kT})$ in the case of α_2 and depends very little on the temperature for α_3 and α_4, in full agreement with the results expected from the transition scheme (Fig. 2).

The vanishing of the RR lines of E_mIC containing more than two holes in strongly deformed crystals is evidence that the formation of such complexes is energywise unfavored in the case of a nondegenerate valence band. By examining the position of the BE_2 line in the RR spectrum of Si(B), corresponding to a transition to the ground state of the EIC, we can trace the decrease of the binding energy of the second exciton $\delta^{(2)}$ in the complex with increasing strain. $\delta^{(2)}$ decreases by an amount close to Δ_v at all pressures up to the vanishing of the RR of E_2IC from the spectrum; this vanishing occurs at $\delta^{(2)} \lesssim 1$ meV, when these complexes become thermodynamically unprofitable. Thus, the binding energy of E_2IC that includes holes only from the ($\pm 1/2$) band does not exceed 1 meV.

The influence of partial lifting of the degeneracy of the conduction band can be traced by investigating the RR spectra of Si deformed along [110] and [100], when 4 and 2 valleys remain, respectively, and the splitting of the valence band is the same as

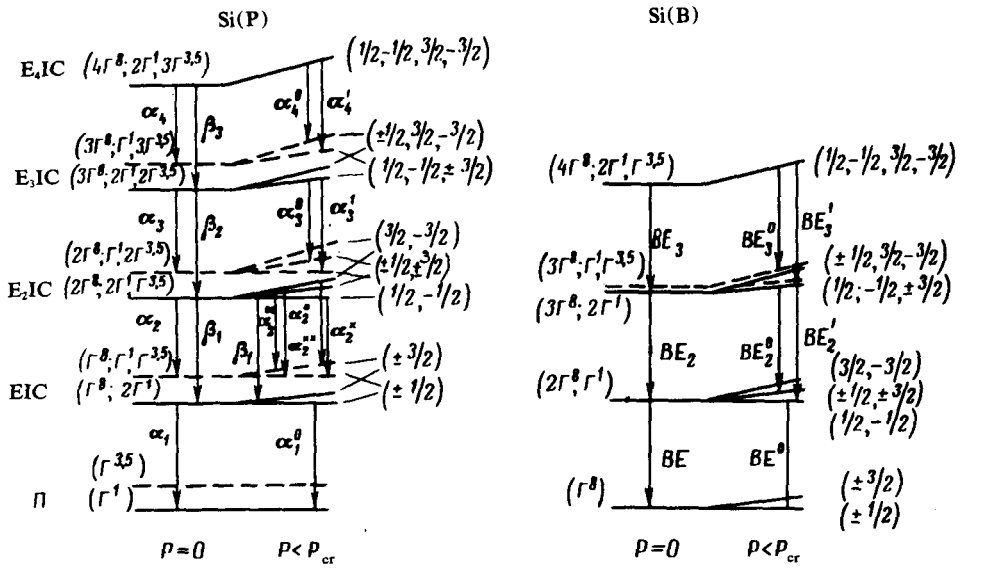

FIG. 2. Transition schemes in recombination of electron-hole pairs in E_mIC in undeformed silicon ($P=0$) and silicon weakly deformed ($P<P_{cr}$) along [111]. The transitions from $(2\Gamma^1,\Gamma^{3.5},4\Gamma^8)$ to $(2\Gamma^1;3\Gamma^8)$ and to $(\Gamma^1,\Gamma^{3.5},3\Gamma^8)$ for Si(B) are marked by the same symbol, since the corresponding RR lines could not be experimentally resolved because of the small splitting of the final state.

at P||[111]. It is seen from the Fig. 3 that in these cases, compared with P||[111], the α spectra of Si(P) do not contain additional lines, even at 10 K, while the RR of Si(B) contain only one additional line BE^*. The line splittings in the doublets are close to Δ_v. This result can be easily explained within the framework of the shell model. The zero-phonon lines α_i correspond to the transitions $(2\Gamma^1,(i-1)\Gamma^{3.5})\rightarrow(\Gamma^1,(i-1)\Gamma^{3.5})$[3]. The state Γ^1 is only doubly degenerate in spin and is not split by the deformation. The states $\Gamma^{3.5}$ are split. This leads to the experimentally observed splitting of the β lines corresponding to recombination of the electrons $\Gamma^{3.5}$ with emission of a phonon. Unfortunately, we were unable to investigate the splitting of the β lines in detail, owing to the superposition, in this spectral region, of the RR lines of the E_mIC with residual boron impurities.

In Si(B) the EIC and E_2IC likewise do not contain the $\Gamma^{3.5}$ electrons. Nor is splitting observed in the BE_3 line, inasmuch as in E_3IC there is only one $\Gamma^{3.5}$ electron. We note that in relatively pure crystals ($N_B \lesssim 10^{13}$ cm^{-3}), owing to the long intervalley relaxation time of the excitons,[10] RR of "hot" bound excitons is observed and correspond to the $\Gamma^{3.5}$ split state. From a comparison of the dependences of the positions of the lines BE and BE^* on the pressure with the picture of the splitting of Γ^1 and $\Gamma^{3.5}$,[11] it follows that the valley-orbit splitting of the states Γ^1 and $\Gamma^{3.5}$ in Si(B) is small (<0.3 meV), as expected in the case of a weakly perturbing acceptor center such as boron.

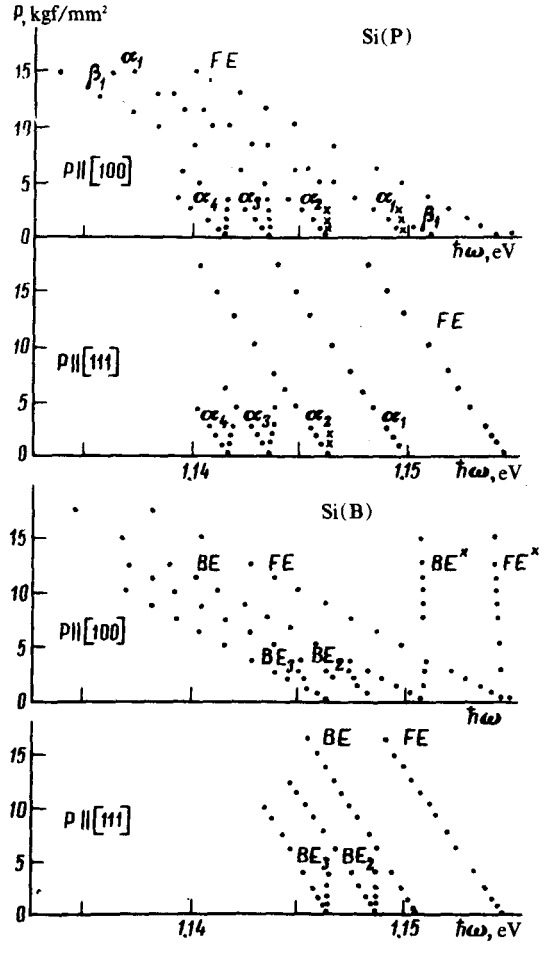

FIG. 3. Splitting of RR lines of EIC in deformation along [111] and [100] at $T=1.8$ K. The additional lines at $T=7$ K are marked by crosses. The energies for β_1, BE_i and FE were obtained by adding $\hbar\omega_{TO}=58.05$ meV to those measured in the TO region of the spectrum.

The binding energy δ of the EIC in Si(P) is greatly decreased by deformation along the axes [110] and [100]. In undeformed Si, Si[111], Si[110] and Si[100] the values of δ are respectively $\delta_0=4.5$; $\delta_{111}=4.3$; $\delta_{110}=3.3$ and $\delta_{100}=2.9\pm0.2$ meV. If the multielectron states are the result of filling of the single-electron states of the neutral donor, then the change of δ is due to the decrease of the valley-orbit splitting as a result of the lifting of the conduction-band degeneracy, and one should expect $\delta_{111}-\delta_{110}\approx\delta_{110}-\delta_{100}$.[11] If the Coulomb repulsion of the electrons located in perpendicular valleys is greatly weakened,[12] then the inequality $\delta_{111}-\delta_{110}\ll\delta_{110}-\delta_{100}$ should be satisfied. It follows from experiment that $\delta_{111}-\delta_{110}$ is somewhat larger than $\delta_{110}-\delta_{100}$, and we assume therefore that this weakening is small. The binding energy of the $\Gamma^{3.5}$ electrons does not depend on the direction and degree of deformation.[11] This agrees with the following properties observed in deformed silicon: a) constancy of the binding energy $\hbar\omega_{FE}-\hbar\omega_{\beta_1}\approx4$ meV of the second exciton in E_2IC (Fig. 3.), and b) constancy of the energy spacings between the α_i lines. It still remains unclear, howev-

er, why, first, $\delta_{111}-\delta_{110}>\delta_{110}-\delta_{100}$, and second, why the splitting between $2\Gamma^1$ and Γ^1 or $\Gamma^{3.5}$ in Si(P) decreases by a factor of two at $\mathbf{P}\|[100]$ rather than by a factor of three as would follow from an analysis of the states of the neutral donor.[11]

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