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IRON IMPURITY RELATED OPTICAL TRANSITIONS IN HgSe:Fe*

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Fe²⁺ crystal field transitions and the heavy hole valence band to the Fe level transitions ($e + \text{Fe}^{3+} \rightarrow \text{Fe}^{2+}$) have been observed and discussed for HgSe doped with iron.

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Relatively little attention has been paid until now to the problem of impurity-related optical transitions for zero-gap semiconductors. The principal reasons were the relatively low values of the resulting absorption coefficients (in comparison with the values corresponding to the usually present interband and intraband transitions) and a very narrow spectral region available for the transmission measurements (limited by the strong absorption mechanisms mentioned above). One of the most interesting impurities in zero-gap semiconductors is Fe in HgSe. For the last 5 years a lot of papers have been devoted to the exciting physical properties of this material (see, e.g. [1-4] and the references therein). However, there exist still unresolved problems due to the lack of some experimental data. For the proper description of the iron-lattice interaction the lattice relaxation energy should be determined or at least experimentally estimated. Another problem could be the

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experimental verification of the results of a recently published theory [5, 6] describing spin-dependent interaction of Γ_8 band electrons with paramagnetic impurities in zinc-blende type semiconductors. The goal of the present work was to get some experimental information about these interactions.

Fig. 1. The structures observed in the low temperature reflectivity spectra for one of our samples HgSe:Fe. The iron concentration is $4.0 \times 10^{19} \text{ cm}^{-3}$, the upper curve corresponds to $T = 5 \text{ K}$, the lower curve corresponds to $T = 50 \text{ K}$. The spectra were taken on a Bruker IFS113 interferometer with a resolution equal to 2 cm^{-1} , the thick samples were mounted on the cold finger of a helium cryostat. The total change of the shown reflectivity coefficient value does not exceed 1% at each temperature.

HgSe is always an n -type semiconductor with a relatively high electron concentration. Fe ions in HgSe are resonant donors. When the Fe concentration is increased above $N_{\text{Fe}} = 4.5 \times 10^{18} \text{ cm}^{-3}$, the Fermi level becomes "pinned" to the Fe level (at low temperatures) and the electron concentration remains constant and equal to $n = 4.5 \times 10^{18} \text{ cm}^{-3}$. It is possible to determine the Fermi energy E_F from the position of the peak (corresponding to the absorption edge) in the reflectivity spectrum taken in the vicinity of E_F . This method has been applied for HgSe:Ga and HgSe:Fe in [7]. In the latter paper the possible influence of the Γ_8 heavy hole valence band on the Fe level optical transitions on the reflectivity spectrum has been discussed. In particular, these transitions produce a supplementary structure in the reflectivity spectra, which in the case of small lattice relaxation energy should be placed in the spectral range below the "principal" peak.

In this paper the supplementary structure in the reflectivity spectra, predicted in [7], has been studied in detail as a function of the temperature and the iron concentration. The dynamic dielectric function formalism for HgSe [8] and the simple model for the Fe impurity related transitions [9] have been used to roughly reproduce the shape and the energy positions of both parts of the whole reflectivity structure. It has been demonstrated that the supplementary structure does not

Fig. 2. (a) "Transmission window" for one of HgSe samples doped simultaneously with Fe and Ga. The iron concentration was $1.4 \times 10^{20} \text{ cm}^{-3}$, the gallium concentration $1.0 \times 10^{19} \text{ cm}^{-3}$, sample thickness $78 \mu\text{m}$. The spectra were taken using the same technique as mentioned in the caption to Fig. 1. Upper curve: $T = 5 \text{ K}$, lower curve: $T = 295 \text{ K}$. The measured spectra have been normalised — the absolute values of the transmission coefficient were determined by the "in-out" method in the monochromatic light. (b) Energy dependence of the absorption coefficient value determined by the "in-out" method for another slice from the same ingot. The sample thickness was $10 \mu\text{m}$, the sample was directly immersed in the helium bath, $T = 1.8 \text{ K}$, the spectral resolution of the spectrometer was 2 cm^{-1} . The dotted curve corresponds to the region of the strong air absorption lines where the accuracy of the measurements is lower than outside of this region. The absorption structures resulting from the Fe^{2+} crystal field transitions are well seen on the absorption background due to the tail of the interband $\Gamma_8^v \rightarrow \Gamma_8^c$ transitions.

exist for HgSe:Ga samples (corresponding to the same high electron concentration equal to about $4.5 \times 10^{18} \text{ cm}^{-3}$), and is more pronounced for samples with higher Fe concentration. The amplitude of this supplementary structure decreases with increasing temperature, but its energy position in practice does not depend on either temperature or Fe concentration (Fig. 1). The energy distance between two parts of the structure in the reflectivity spectra within an accuracy of the order of a few meV corresponds to the energy resulting from the possible curvature of the Γ_8 heavy hole valence band. Thus, the lattice relaxation energy has been roughly estimated as being close to zero (at least not higher than about 30 cm^{-1} (a few meV)).

For the highly doped *n*-type samples the low energy edge of the "transmission window" in the infrared is determined by the plasma edge, while the interband $\Gamma_8^v \rightarrow \Gamma_8^c$ transitions give the high energy "cut-off". It was possible to shift the "transmission window" into the spectral region of the expected Fe^{2+}

crystal field transitions [10, 11] by simultaneous HgSe doping with Fe and Ga. The results obtained are shown in Fig. 2. The measured absorption spectrum consists of two parts. The first strong peak lies at $(2423 \pm 3) \text{ cm}^{-1}$ and corresponds to the zero-phonon transitions. The maximum absorption coefficient is about 450 cm^{-1} , the full width at half maximum is about $(85 \pm 3) \text{ cm}^{-1}$. The second broad bump lies in the spectral range $2540\text{--}2650 \text{ cm}^{-1}$ and corresponds to the optical phonon-assisted transitions [12, 13]. The peak at 2423 cm^{-1} is not split into the separated zero-phonon transitions. This can be due to the broadening of the 5T_2 excited Fe^{2+} state resulting from the p - d hybridization [5, 6]. However, this broadening cannot be higher than about $20\text{--}30 \text{ cm}^{-1}$.

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