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ALLOCATION AND PROPERTIES OF IRON STATES IN $\text{Cd}_{1-x}\text{Fe}_x\text{Te}$ IN FORBIDDEN GAP ENERGY RANGE*

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The use of different experimental methods (reflectivity, absorption, photoconductivity and cathodoluminescence) allowed us to confirm the existence of the deep donor-like state of iron and present allocation and properties of the iron states in $\text{Cd}_{1-x}\text{Fe}_x\text{Te}$ ($0 \leq x \leq 0.05$) at 300 K and 77 K in the forbidden gap energy range. It was concluded that the increase in width of the forbidden gap with the change of temperature from 300 K to 77 K leads mainly to the rise of the energy distance between the donor-like iron state 5E and the bottom of the conduction band.

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The semiconducting compound $\text{Cd}_{1-x}\text{Fe}_x\text{Te}$ belongs to the family of diluted magnetic semiconductors [1, 2]. The optical properties of this compound have been studied using absorption [3, 4], reflectivity [5, 6], and photo-EPR measurements [7]. On the basis of the results of these measurements there has been recognized a state of iron, identified as the so-called deep donor and its ionization energy related to the transition $\text{Fe}^{2+}(d^6) \rightarrow \text{Fe}^{3+}(d^5)$ has been calculated to be 1.45 eV with respect to the bottom of the conduction band minimum (CBM). The existence of the donor-like state and its ionization energy value has been confirmed [6, 8].

Our reflectivity (RE), transmission and photoconductivity (PC) measurements procedure and experimental apparatus were described earlier [9]. The PC measurements were taken using modulated beam light (modulation frequency equal to 11 Hz) in the constant collecting electric field. In the cathodoluminescence (CL) measurements the employed electron beam energy was 10 keV. Using the calibrated dependence of the lattice constant versus chemical composition presented in paper [6], the iron concentrations x were determined.

Reviews of the E_0 maxima energy positions obtained from the RE measurements and E_{pc} PC signal as a function of iron concentration x at 300 K (RT) and

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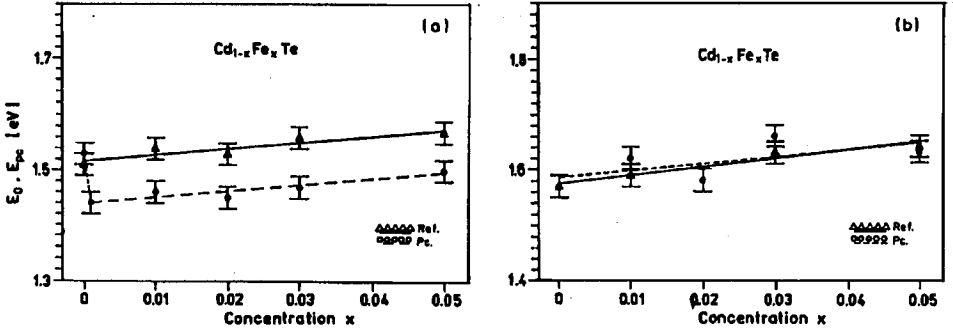


Fig. 1. The dependence of the energy position of E_{pc} and E_0 maxima on iron concentration at 300 K (a) and 77 K (b).

77 K (LNT) are shown in Fig. 1. The E_0 energy value agrees, to the accuracy of exciton bond energy, which for CdTe is approximately 20 meV, with the forbidden energy gap value [11]. The dependence of energy position E_0 on iron concentration x is linear and equals $E_0^{RT} = (1.13 \pm 0.28)x + (1.517 \pm 0.008)$, $E_0^{LNT} = (1.44 \pm 0.26)x + (1.575 \pm 0.008)$ at RT and LNT, respectively. As it can be seen, at RT, introduction of small amount of iron into the CdTe matrix changes rapidly the energy position of the PC maximum (E_{pc}) towards lower energies. Further increase in iron content in crystal is followed by a linear rise of the E_{pc} value according to the equation $E_{pc}^{RT}(x) = (1.12 \pm 0.24)x + (1.438 \pm 0.006)$. At LNT, an introduction of even small amount of iron ($x = 0.001$) does not result in a rapid change in energy position of E_{pc} . The fitted linear dependence has the following parameters: $E_{pc}^{LNT} = (1.12 \pm 0.4)x + (1.589 \pm 0.02)$. The CL spectra obtained for mixed crystals $Cd_{1-x}Fe_xTe$ at LNT are presented in Fig. 2. In the spectrum for iron concentration $x = 0.01$ three peaks labeled E_a , E_b and E_c can be seen. Energy positions of these peaks are given in Table. An increase in iron concentration, at RT results in a shift of the onset of the rise of the dependence absorption coefficient $\alpha(E)$ towards lower energies, whereas at LNT, apart from this regularity a pre-edge maximum appears at the energy 1.38 ± 0.02 eV. In RE spectra there has also been observed a distinct maximum occurring before E_0 , at energies 1.40 eV (at RT) and 1.45 eV (at LNT).

For crystal field parameters characteristic of CdTe [3, 10], one can find energy distances of ${}^5E \rightarrow {}^5T_2$ (2500 cm^{-1}) and ${}^5E \rightarrow {}^3T_1$ (11200 cm^{-1}) transitions within Fe^{2+} . If the ground state of iron is placed about 0.1 eV above the valence band maximum (VBM), the next excitation states should be 0.31 eV and 1.39 eV above the ground state, as it is shown in Fig. 3. The obtained results can be consistently explained by assuming the allocation of iron states presented in Fig. 3. For pure CdTe, E_0 and E_{pc} energy values agree well within experimental error. The rapid jump of E_{pc} value at RT towards lower energies at about 0.1 eV with the introduction of even small amount of iron ($x = 0.01$) should be thus associated with the process of absorption from the 5E state of iron to CB, while in pure CdTe, PC seems to be determined by the $VB \rightarrow CB$ transition [12]. As at RT the

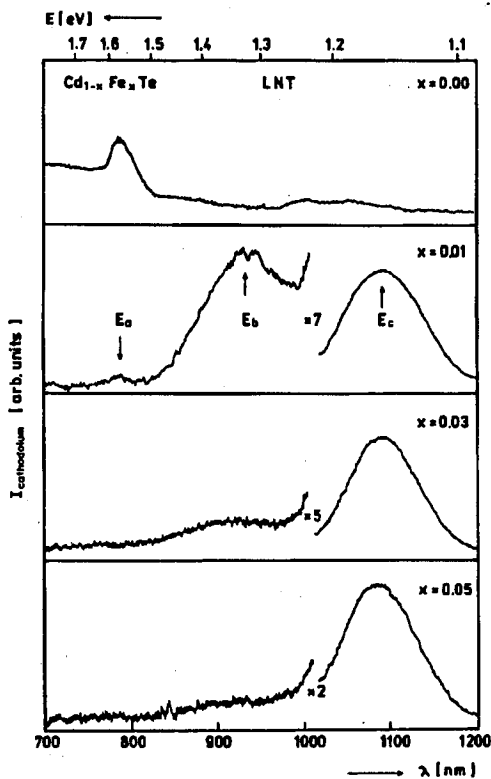


Fig. 2. The cathodoluminescence spectra for $Cd_{1-x}Fe_xTe$ obtained at 77 K.

TABLE
Energy positions of the maxima E_a , E_b and E_c observed in cathodoluminescence spectra for $Cd_{1-x}Fe_xTe$ at 77 K.

Concentration x	E_a [eV]	E_b [eV]	E_c [eV]
0.00	1.57 ± 0.02	—	—
0.01	1.57 ± 0.03	1.33 ± 0.02	1.13 ± 0.01
0.03	—	?	1.14 ± 0.01
0.05	—	—	1.14 ± 0.01

slopes of E_0 and E_{pc} are, within the experimental error, the same, this suggests that the final state in both processes is CBM since the distance between VBM and the 5E state remains practically the same. This result confirms behavior of a bump appearing below the E_0 value in the RE spectra after introduction of iron into the CdTe matrix and appearing of a pre-edge maximum in the $\alpha(E)$ dependence, only at LNT. Since the probability of thermal excitation of electron between VBM and the 5E state of iron is about 4 orders smaller at LNT than at RT, then the PC process seems to be determined by $VB \rightarrow CB$ transitions [12]. It is also worth noting that at LNT the 3T_1 excitation state of iron is localized very

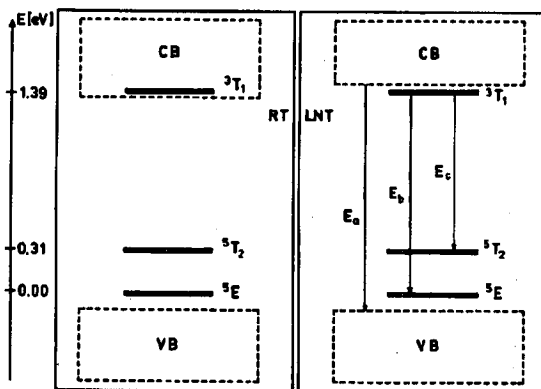


Fig. 3. The allocation of iron states in the CdTe matrix in the forbidden gap region at 300 K and 77 K. At 77 K the interpretation of maxima observed in the cathodoluminescence spectra is presented.

close to the bottom of conduction band and may act as a holding or recombination trap (Fig. 3). Interpretation of the E_a , E_b , E_c maxima observed in the CL spectra for LNT has been presented in Fig. 3. Increase in iron concentration leads to the increase in density of initial and final states in the ${}^3T_1 \rightarrow {}^5T_2$ (E_c) and ${}^3T_1 \rightarrow {}^5E$ (E_b) processes. Taking into account the allocation of final state energies of these transitions on the energy scale, one can expect that lower energy interval transitions will become dominating at the set number of thermalized electrons, resulting in disappearance of the E_b (${}^3T_1 \rightarrow {}^5E$) maximum, which has, in fact, been observed.

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