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Iodine-impurity level in MBE-grown $Cd_{1-x}Mn_xTe$

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We present results of the Hall effect and resistivity measurements performed at a hydrostatic pressure up to 1.45 GPa on molecular beam epitaxy-grown CdTe and $Cd_{1-x}Mn_xTe$ layers doped with iodine. Our data provide an evidence that in CdTe:I the iodine impurities introduce electronic states resonant with the conduction band, at about 320 meV above its edge. The energy of this state decreases in $Cd_{1-x}Mn_xTe$ at a rate of 11 meV per 1% of Mn molar fraction. The iodine level reveals metastable properties at low temperatures in close analogy to other donors in CdTe and to *DX* centers in GaAs. The experimental data are analyzed in terms of positive and negative *U* (electron-electron on-site correlation energy) models of the iodine impurity charge state. Both models reasonably well reproduce the experimental behavior. [S0163-1829(99)08719-6]

I. INTRODUCTION

Progress of epitaxial growth techniques of the II–VI semiconducting compounds, stimulated by their possible applications in a variety of optoelectronic devices including blue lasers, has focused new interest on donor dopants and their deep localized states. Investigations of molecular beam epitaxy (MBE)-grown layers of II–VI compounds doped with Cl, Br, and In (Refs. 1–6) revealed a general problem appearing in these semiconductors, namely that an intentional doping usually leads to a formation of compensating defects or defect complexes. Higher electron concentrations have been recently achieved by using iodine as an *n*-type dopant.[7–9] This particular choice appears to be very efficient in producing *n*-type CdTe, $Cd_{1-x}Mn_xTe$, $Cd_{1-x}Mg_xTe$, and $Cd_{1-x}Zn_xTe$ layers with the free-electron concentration up to 10^{19} cm^{-3}, i.e., by about one order more heavily doped than it is possible in the case of other dopants mentioned above. Also, the use of iodine in modulation-doped CdTe/CdMgTe heterostructures resulted in fabrication of two-dimensional (2D) electron gas with the highest mobility reported so far in wide-gap II–VI materials.[9,10] In contrast to the other dopants mentioned above the iodine deep level has not been observed.

The aim of our work was to search for the iodine impurity level in CdTe:I and $Cd_{1-x}Mn_xTe$:I and to study its properties. It is expected that iodine should have properties similar to other donors like Cl, Ga, Br, and In, which, apart from hydrogenic states, create also highly localized states in II–VI binary compounds[3,8,11–15] and their alloys.[16–20] At ambient pressure these deep levels are in CdTe resonant with the conduction band with their energies ranging from about 0.05 eV for chlorine to 0.26 eV for bromine, both with respect to Γ_6 minimum. At low temperatures these states exhibit metastable properties analogous to those of *DX* centers in GaAs and $Ga_xAl_{1-x}As$.[21,22] From the physical point of view one of the most interesting problems related to *DX* and *DX*-like centers was the charge state of these defects when occupied by electrons. The problem is usually considered in terms of either positive or negative Hubbard correlation energy *U*.[23,24] Centers with both positive and negative *U* have been reported in the literature. For example, certain localized states in GaAs reveal a negative *U* character (e.g. Refs. 25–27 and references therein), while experimental data obtained for nominally undoped *n*-InSb could be understood only assuming that the deep donor states have a positive correlation energy *U*.[28,29] In the case of iodine impurity in CdTe theoretical calculations of Park and Chadi[30] predict three different types of *DX*-like centers, all having negative Hubbard energy *U*. Among these three types of states, the most stable one (labeled DX_1) has a microscopic structure similar to that of a column VI impurity in III–V semiconductors. However, to our knowledge, there has been no experimental confirmation of these expectations.

In the present paper, we based our investigations on electrical measurements performed under hydrostatic pressure which proved to be a very useful tool in studies of similar type of defects. Since the pressure coefficient of the Γ_6 conduction-band minimum is expected to be considerably greater than that of the localized level due to I impurity, as is the case of other donors (e.g., Refs. 11 and 15), one could also expect a relative pressure-induced downward shift of the defect level with respect to the bottom of the conduction band. This can lead to a trapping of electrons by impurity centers at sufficiently high pressures. Previous hydrostatic pressure experiments performed on bulk CdTe:I did not reveal any pressure-induced changes of the free-electron concentration.[11] This result could be understood assuming that the iodine resonant level was either located too high in the conduction band to be occupied even at the highest applied pressure or this dopant did not form any localized states. In the present study we investigated CdTe:I layers with extremely high concentration, namely 1.4×10^{19} cm^{-3} (by one order of magnitude greater than those used previously[11]), as well as $Cd_{1-x}Mn_xTe$:I samples. In the latter case, in analogy to *DX*-centers in $Ga_xAl_{1-x}As$, we could expect that the impurity level should be located closer to the bottom of the conduction band than in CdTe, due to the

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TABLE I. Parameters characterizing the samples used in the experiments.

Sample	Mn molar fraction x	Iodine concentration $N_{ISIMS}(\mathrm{cm}^{-3})$	Electron concentration $n_H(\mathrm{cm}^{-3})$	Compensation ratio k_C	Hall mobility $\mu(\mathrm{cm}^2/\mathrm{Vs})$
CdTe:I	0	2.5×10^{19}	1.4×10^{19}	0.28	360
$Cd_{0.93}Mn_{0.07}Te:I$	0.07	2.5×10^{19}	5.3×10^{18}	0.66	220
$Cd_{0.88}Mn_{0.12}Te:I$	0.12	1.5×10^{19}	4×10^{18}	0.58	73
$Cd_{0.80}Mn_{0.20}Te:I$	0.20	1.5×10^{19}	1×10^{18}	0.88	62

increase of the energy gap with the molar fraction of Mn.

The paper presents results that demonstrate for the first time that the iodine impurity DX-like localized state does exist. We determine the energy of this level in $Cd_{1-x}Mn_xTe$ as a function of x and we analyze the defect metastable properties.

II. EXPERIMENTAL METHODS AND RESULTS

A. Experiment

In our experiments we used iodine-doped n-type CdTe and $Cd_{1-x}Mn_xTe$ (for x equal to 0.07, 0.12, and 0.20) layers grown by molecular beam epitaxy (MBE) at the substrate temperature equal to 250 °C. Elemental sources of Cd (7N), Te (7N), and Mn (5N) were used while the doping was performed from a compound source containing ZnI_2 (5N). CdTe and CdMnTe layers 0.5-μm thick were grown on semi-insulating (100) GaAs substrates covered with 10 Å of ZnTe followed by $3\div4$-μm thick buffer of undoped CdTe. Determination of the molar fraction of manganese in $Cd_{1-x}Mn_xTe$ layers was based on an earlier calibration of MBE processes involving measurements of the energy of the free exciton luminescence. The total concentration of the iodine impurities introduced into the layers was measured by secondary ion mass spectroscopy (SIMS) technique.

The Hall effect and resistivity measurements were performed as functions of hydrostatic pressure up to 1.45 GPa in the temperature range from 77 to 300 K. We used high-pressure equipment with helium gas as the pressure transmitting medium which allowed us to change the value of the pressure acting upon a sample at a constant low temperature. An infrared GaAs light emitting diode (LED) was also mounted in the pressure cell, which made the (persistent) photoionization of investigated impurity centers possible. Ohmic contacts were formed by annealing indium pellets in vacuum at 180 °C for about 1 min. Hall bars were defined by indenting the surface of the layers with a steel needle. Parameters characterizing our samples, i.e., Hall concentration n_H and Hall mobility μ measured at $T=190$ K, are listed in Table I.

B. Results

The variation of the Hall concentration n_H with pressure measured at $T=190$ K for all our layers is presented in Fig. 1. One can see that the pressure induces a decrease of the free-electron concentration. However, the magnitude of the changes depends strongly on the manganese molar fraction, x. For the sample with $x=0.20$ the electron concentration decreases from 1×10^{18} cm^{-3} at ambient pressure down to 3.8×10^{16} cm^{-3} at $p=1.1$ GPa. In the sample with Mn molar fraction equal to 12% the decrease of n_H is less pronounced. The free-electron concentration remains practically constant up to about 0.7 GPa and only for higher pressures a decrease of n_H is observed. For the layers with $x=0.07$ and $x=0$ the variation of n_H under hydrostatic pressure is very weak. The total change of the free-electron concentrations amounts to only about 20% and 10% in the sample with $x=0.07$ and $x=0$, respectively.

The above results could be understood assuming that the iodine impurity gives rise to a level, which at $p=0$ GPa is resonant with the conduction band and thus provides electrons to the conduction band. As the pressure is increased, the energy of the impurity level decreases relatively to the Γ_6 minimum. At sufficiently high pressures, when the level approaches the Fermi energy, the free electrons become trapped by the impurity centers, which is observed in the Hall effect experiments as a drop of the free-electron concentration. The effect of alloying is somehow similar to that of pressure—the energy of the level decreases with Mn molar fraction due to alloying-induced increase of the energy gap. In the CdTe:I sample the impurity level lies so high in the conduction band that even for the Fermi energy of about $E_F\approx210$ meV (at $p=0$) above the bottom of the conduction band the applied pressure is not high enough to produce any visible freezout. Obviously, in $Cd_{0.80}Mn_{0.20}Te:I$ sample the iodine level is much closer to the Γ_6 minimum as well as to the Fermi energy because the decrease of the number of free electrons becomes substantial at relatively low pressures. As we shall see, at the highest applied pressures the level even enters the forbidden gap in this sample.

The pressure dependencies of the Hall mobility measured at $T=190$ K in all our samples are shown in Fig. 2. In the case of CdTe:I and $Cd_{0.93}Mn_{0.07}Te:I$ samples only a very weak (of the order of 5% at the highest pressure) and nearly linear decrease of the mobility with pressure was observed. Such a variation can be qualitatively understood in terms of the pressure-induced increase of the effective mass. On the other hand, in $Cd_{0.80}Mn_{0.20}Te:I$ sample the decrease of the mobility is much more pronounced reaching about 40%. In the case of $Cd_{0.88}Mn_{0.12}Te:I$ layer the mobility is almost constant for the pressure lower than about 0.8 GPa and then it decreases by about 14% for $p>0.8$ GPa.

As mentioned, the above results were obtained at 190 K. At lower temperatures (lower than a critical temperature T_C) the experimental results are quite different. In all our samples clear manifestations were observed of metastable occupation of the iodine impurities (such as persistent photoconductivity), typical for DX-like centers. The results presented in Fig.

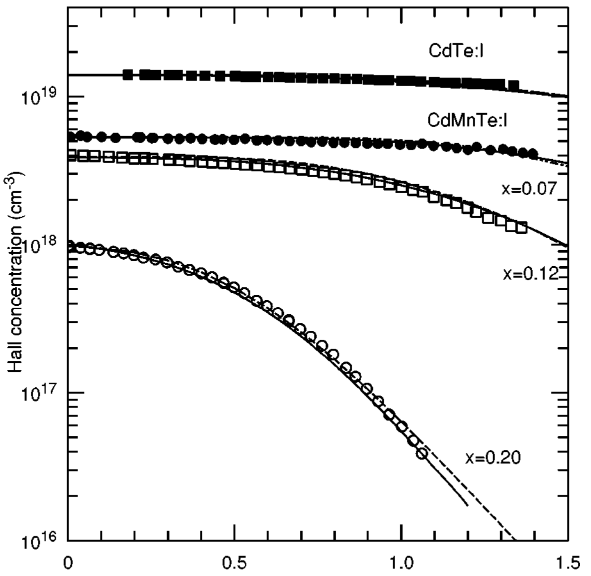

FIG. 1. Hall concentration versus pressure measured at $T = 190$ K. Solid and dashed lines are theoretical calculations (see text) within the positive and negative U models of the impurity center, respectively.

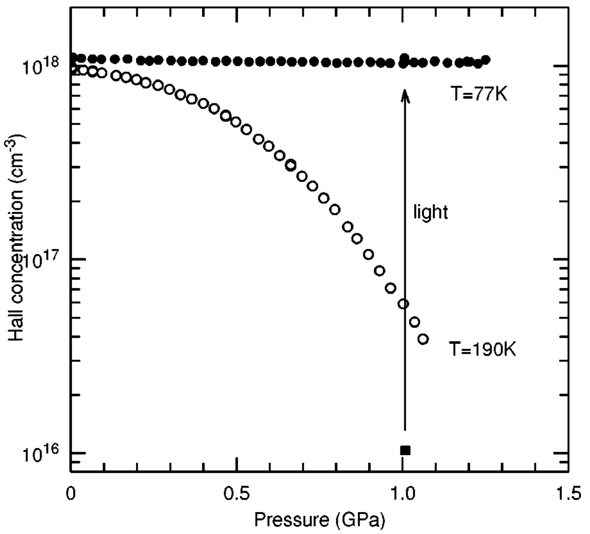

FIG. 3. Hall concentration in $Cd_{0.80}Mn_{0.20}Te$:I as a function of pressure applied at $T = 190$ K (open circles) which was later released at $T = 77$ K (full circles) after illumination. The point-full square was measured at 77 K before illumination, but after application of pressure at 190 K and then cooling the sample down to 77 K at $p = 1$ GPa. The arrow shows the increase of the Hall concentration after illumination at 77 K and $p = 1$ GPa.

3, obtained for $Cd_{0.80}Mn_{0.20}Te$:I, are qualitatively the same in the remaining samples. As we described, for $T > T_C$ the increase of pressure leads to lowering of the free-electron concentration. If the temperature is then lowered below T_C (while the high pressure remains applied), the occupation of iodine impurities is frozen and observation of different values of the free-electron concentration at the same external conditions is possible. For example, a few minutes of illumination by LED induces an increase of n_H, which persists even if the pressure is released. On the other hand, when the temperature is raised after persistent photoionization of the iodine impurities, still with the high pressure applied to the sample, one can observe the recovery of the equilibrium occupation of I donors. This can be seen in the temperature transients shown in Figs. 4(a) and 4(b) as a steplike decrease of n_H, position of which defines T_C. As it is seen from Fig. 4, T_C is slightly different in CdTe:I and $Cd_{0.80}Mn_{0.20}Te$:I. This can probably be attributed to different value of the Fermi energy in these two samples—the Fermi level in CdTe:I is much higher, which makes it easier for the electron to overcome the capture barrier leading in consequence to an effectively lower T_C. The above results are in close analogy to those seen in CdTe:In (Refs. 14 and 15) as well as in GaAs heavily doped with Si, Te, and Se.[21,22]

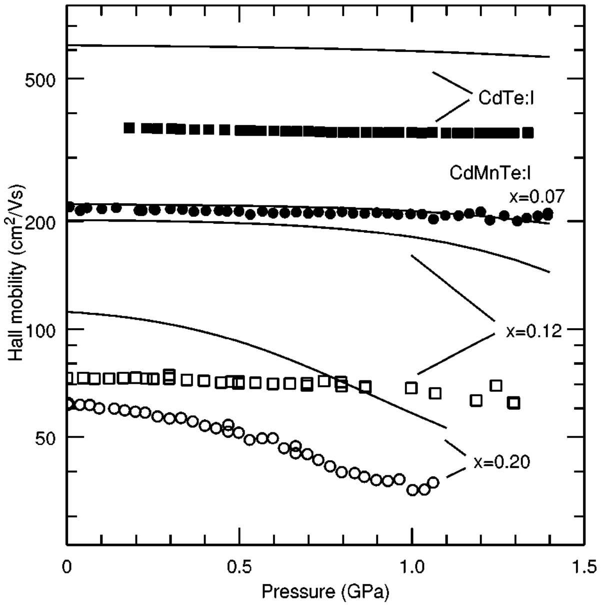

FIG. 2. Hall mobility as a function of pressure measured at $T = 190$ K. Solid lines are theoretical calculations performed within positive U model of the impurity center.

III. DISCUSSION

A. Hall concentration

Our experimental results provide an unambiguous proof of the existence of the iodine-related level that is degenerate with the conduction band and that possesses metastable properties at $T < T_C$. In order to determine the thermal ionization energy of the level and its pressure shift we performed calculations assuming either a single or double occupation of the state by electrons (i.e., assuming either the positive or negative on-site Hubbard correlation energy U). In both cases we assumed that the I-level is in thermal equilibrium with the conduction band at temperatures higher than T_C and can be described by δ-like density of states. We have also assumed that the conduction band is spherical with a parabolic dispersion and neglected the effects of the subsidiary L and X minima, which are located well above the Γ minimum even at the highest pressures. Since the measurements of exciton energy in a magnetic field in $Cd_{1-x}Mn_xTe$ showed that for this ternary semiconductor system the effective mass in the conduction band is practically independent

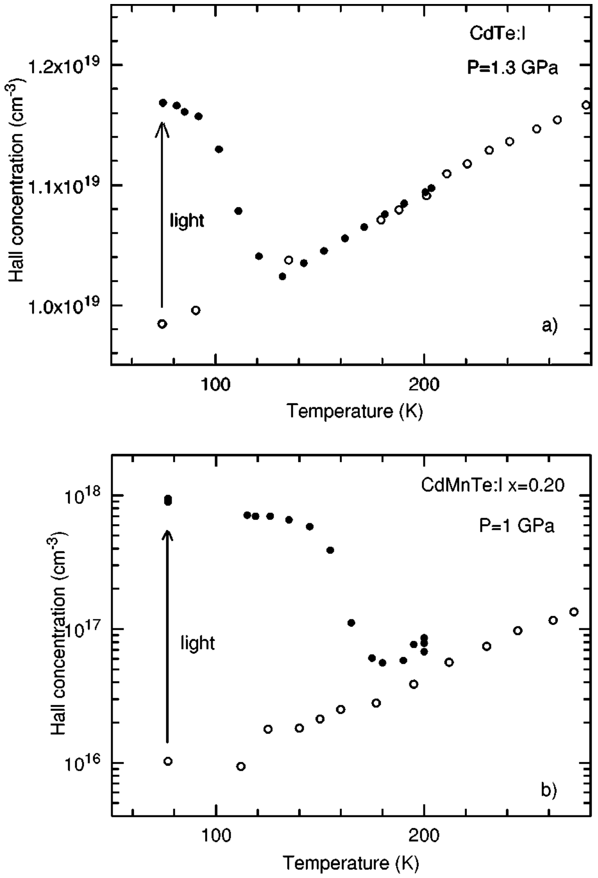

FIG. 4. Temperature transients of the Hall concentration measured for various metastable occupations of the localized iodine state in: a) CdTe:I, b) $Cd_{0.80}Mn_{0.20}Te:I$. The points-open circles were measured during cooling the samples down, while full circles during heating them up after illumination performed at 77 K. The arrows show the increase of the Hall concentration after illumination.

of Mn content,[31] therefore in our calculations we took the same value of the effective mass $m^* = 0.1m_0$ for all the samples considered. This value corresponds to the effective mass of CdTe at ambient pressure.[32] We have assumed that the variation of the m^* with pressure is proportional to the pressure coefficient of the gap, $\partial E_g/\partial p$, i.e., $m^*(p) = m^*(1 + 1/Eg \cdot \partial Eg/\partial p \cdot p)$. This correction of the effective mass is relatively small, and at the highest applied pressure of 1.4 GPa it amounts to about 7.5%.

The concentration of iodine impurities N_I as well as the concentration of acceptors, N_A, have been evaluated in the following manner. For all our samples the free-electron concentration was almost constant at low pressures, which meant that practically all the iodine impurity centers were ionized at ambient pressure, thus $n_H(p=0) = N_I - N_A$. Then we adopted the self-compensation concept originally used for CdTe that intentional *n*-type doping is generally accompanied by a formation of compensating complexes each of them containing the dopant atom and some native defect.[33,34] Therefore, we have assumed that the total concentration of the iodine impurities measured by SIMS is equal to $N_{I\,SIMS} = N_I + N_A$. This has enabled us to calculate the values of N_I and N_A as well as the compensation ratio $k_C = N_A/N_I$ listed in Table I.

The charge of the iodine centers occupied by electron depends on the sign and the value of electron-electron correlation energy U. In the case of the one-level positive U model the impurity center can trap only one electron changing its charge state from $(+)$ to neutral (0). However, for the negative U model generally one has to consider three possible charge states of an impurity: positive, neutral, or negative. Coexistence of all the three charge states was reported to occur, e.g., for Ge impurity in GaAs.[27,35] On the other hand, if the energy U has a large negative value $(|U| \gg k_B T)$, the neutral charge state cannot be achieved. Since our data reveal the existence of only one level, trapping free electrons, it means that, if really $U<0$ occurs, we are dealing with the latter case, i.e., under hydrostatic pressure the center can simultaneously trap two electrons changing its charge state directly from $(+)$ to $(-)$.

The charge neutrality equations for both considered models of the impurity are the following: $n + N_A = N_I^+$, and $n + N_A + N_I^- = N_I^+$ for $U>0$ and $U<0$ case, respectively, where N_I^+ and N_I^- stand for positively and negatively charged I centers (see appendix). We have assumed linear variation of the thermal ionization energy of the iodine level with hydrostatic pressure and with molar fraction of Mn: $E_I(p,x) = E_I(0) + \partial E_I/\partial p \cdot p + \partial E_I/\partial x \cdot x$. Thus the neutrality equations contain only three unknown parameters, which were fitted to obtain the best agreement between the calculated and measured $n_H(p)$ dependencies. The fittings were performed for three CdMnTe:I samples. For CdTe:I the pressure-induced decrease of the free-electron concentration was too small to permit a reliable fitting procedure. The results of the calculations are shown in Fig. 1 as solid and dashed lines for $U>0$ and $U<0$ models, respectively. It is clear that both models reproduce experimental $n_H(p)$ dependencies equally well (the dashed and solid lines almost coincide) and, moreover, with similar values of the fitted parameters, namely:

$$E^{+/0}(p,x) = 329 \text{ meV} - 102 \text{ meV/GPa} \cdot p$$
$$- 1140 \text{ meV} \cdot x \quad \text{for } U>0$$

and

$$E^{-/+}(p,x) = 316 \text{ meV} - 93 \text{ meV/GPa} \cdot p$$
$$- 1130 \text{ meV} \cdot x \quad \text{for } U<0.$$

The energies are given with respect to the Γ minimum of the conduction band. The thermal energy $E_I^{-/+}$ (for $U<0$) is given per one electron. Both values of the pressure coefficients agree well with the pressure derivatives of the energy levels of other donors in CdTe (see, e.g., Ref. 15) and with corresponding theoretical predictions.[30]

Although in the calculations the compensation of the samples was determined from the SIMS data, we have checked that thermal ionization energies and $\partial E_I/\partial x$ are practically independent of the sample compensation as well as the model of the impurity charge. However, the fittings performed within $U>0$ model for the $Cd_{0.80}Mn_{0.20}Te$:I sample showed that the pressure coefficient varied almost twice with the compensation being changed from $k_C = 0$ to $k_C = 0.9$ contrary to $U<0$ model where $\partial E_I/\partial p$ was independent of the compensation. This suggests that the problem of the charge state of the iodine impurity center can be experimentally solved by means of pressure studies of specially chosen samples, i.e., with low compensation and Mn content $x \approx 0.20 \div 0.25$.

B. Upper limit of the free-electron concentration

The existence of the donor level degenerate with the conduction band introduces an upper limit for the free-electron concentration in CdTe and $Cd_{1-x}Mn_xTe$ heavily doped with iodine due to the pinning of the Fermi energy to the impurity level. For CdTe the Fermi energy $E_F = E_I$ corresponds to a very high value of the free-electron concentration equal to about 3×10^{19} cm^{-3}. However in $Cd_{1-x}Mn_xTe$ the impurity level is closer to the bottom of the conduction band. This makes upper limit of n_H smaller in the ternary material. In $Cd_{0.80}Mn_{0.20}Te$ the limit can be estimated to be about 5×10^{18} cm^{-3}. For Mn molar fraction $x \approx 0.30$, the iodine level enters the gap, which corresponds to a maximum free-electron concentration (at room temperature) $n \approx 2 \times 10^{17}$ cm^{-3} only. It should be pointed out that, since in samples with the iodine concentration close to (or above) this upper limit some of I impurities are already occupied by electrons even at ambient pressure, one should expect in such a case undesirable, metastable properties at low temperature, e.g., persistent photoconductivity. It means that the upper limit of dopant concentration should not be exceeded. Nevertheless, iodine is still the best known donor dopant in CdTe and $Cd_{1-x}Mn_xTe$ $(x < 0.30)$ materials.

C. Electron mobility

In this section we focus on qualitative understanding of the main features of the mobility, μ, observed in the experiments. We shall analyze the change of μ with Mn molar fraction in ternary $Cd_{1-x}Mn_xTe$:I layers. Then we shall discuss the dependence of the mobility on hydrostatic pressure. This dependence is quite weak even in $Cd_{0.80}Mn_{0.20}Te$:I for which the pressure-induced variation of the free-electron concentration reaches almost two orders of magnitude. The natural explanation of the mobility dependence on Mn content is the chemical disorder scattering. Treating the potentials introduced by Cd and Mn atoms as deviations from an average potential of a virtual crystal one obtains for the relaxation time of a carrier in a parabolic and spherical conduction band[36]

$$\tau_k = \frac{\pi \hbar^3}{x(1-x) k m^* N V^2},$$

where k is the wave vector, N-the number of cations per unit volume, and the parameter V is the matrix element of the difference between atomic potentials of Cd and Mn atoms, calculated for s-like Bloch wave function in the conduction band. The relaxation time τ_k decreases with Mn content for $x < 0.5$. It also depends on the free-electron concentration via the wave vector k, increasing with the decrease of n_H.

In the calculations we used the procedure described in Ref. 37 taking into account beside the scattering mechanism mentioned above, the scattering by screened Coulomb potentials of ionized impurities and the scattering by phonons. The concentration of the ionized centers, N_i was evaluated based upon the SIMS data and our experimental values of the free-electron concentration. Within the positive U model it was equal to $N_i = N_A + N_I^+(p)$ while in the case of the negative U model, the number of charged centers was pressure independent, being equal $N_i = N_A + N_I = N_{ISIMS}$. In our calculations the only unknown parameter is the matrix element V. Having in mind that the theoretical mobility should not be lower than its experimental values, we found that parameter V cannot exceed 2.8×10^{-22} eV cm^3. This value is of the same order as for other ternary semiconductors (see, e.g., Ref. 36 and references therein) and corresponds to the best agreement between calculated curves and experimental points for the sample with $x = 0.07$. For other samples the calculated values of the mobility visibly exceed the experimental data, which is illustrated in Fig. 2—solid lines were calculated within $U > 0$ model using $V = 2.8 \times 10^{-22}$ eV cm^3.

This result means that in our samples also other scattering mechanisms, beside those considered above, were probably active. They can include scattering by neutral impurities or/and dislocations etc., which can further reduce absolute values of the mobility. Nevertheless, in spite of the mentioned discrepancy, our calculations reproduce qualitatively the main features of the experimental data. In particular, we can explain the decrease of the absolute value of the mobility with the molar fraction of Mn in terms of the disorder scattering. This scattering channel makes, in particular, the mobility of the sample with $x = 0.20$ distinctly smaller than that in CdTe:I sample although the former contains less ionized impurities.

Our theoretical calculations describe properly, both in $U > 0$ and $U < 0$ models, a relatively weak dependence of the mobility on pressure. For CdTe:I and $Cd_{0.93}Mn_{0.07}Te$:I samples a very weak decrease of the mobility with pressure was predicted in agreement with the experimental data. The pressure dependencies are mainly due to pressure-induced increase of the effective mass. For $Cd_{0.80}Mn_{0.20}Te$:I and $Cd_{0.88}Mn_{0.12}Te$:I samples the relative changes of the mobility with pressure are shown in Fig. 5. Solid and dashed lines correspond to the calculations within $U > 0$ and $U < 0$ model, respectively. Both models reproduce well the weak decrease of the mobility with pressure. This fact is connected with a high compensation of the samples. In such a case the variation of the mobility upon hydrostatic pressure is mainly governed by the effect of the screening of Coulomb potentials. The screening by free electrons weakens with decreasing their concentration (and not with changes of N_i). Within the positive U model this effect of screening is much stronger than that related to pressure-induced decrease of the concentration of iodine ionized impurities, which become neutral after trapping electrons.

High-compensation ratio explains also a very small difference between the calculations within both models (shown by solid and dashed curves in Fig. 5, respectively). This is particularly true in the case of $Cd_{0.80}Mn_{0.20}Te$:I sample, which has the largest compensation ratio, i.e., $k_C = 0.88$. For the sake of completeness we also performed analogous numerical analysis of the mobility taking additionally into account the scattering by neutral impurities. To do this we have to introduce new fitting parameters, one for each sample. Not surprisingly, one can reproduce then very well both the ab-

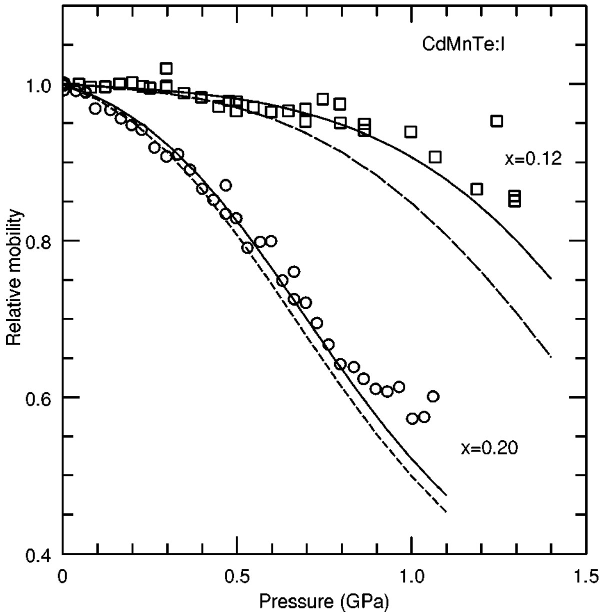

FIG. 5. Relative mobility in $Cd_{0.80}Mn_{0.20}Te:I$ and $Cd_{0.88}Mn_{0.12}Te:I$ samples. Solid and dashed lines are the theoretical calculations performed within the positive and negative U models, respectively (see text).

solute values of the mobility in all the investigated samples and their pressure dependencies. However, the conclusions following from such analysis are not different from those above: because of high compensation of our samples it is impossible to distinguish unambiguously between the $U>0$ and $U<0$ models of the iodine impurity centers.

IV. CONCLUSIONS

The main conclusion of our paper is that iodine impurity in MBE-grown CdTe:I and $Cd_{1-x}Mn_xTe:I$ layers introduces the electronic level, which is resonant with the conduction band. The level reveals DX-like character. The observed effects of persistent photoconductivity and the metastable occupation of the level at low temperatures ($T<T_C\approx 120 \div 160$ K) induced by hydrostatic pressure are in close analogy to those seen for other donors in CdTe as well as in GaAs heavily doped with donors. However, based on our experimental data we are not able to unambiguously distinguish between $U<0$ and $U>0$ cases. Both models can reproduce our experimental data of the free-electron concentration as well as of the mobility. Both models render similar values of the fitted impurity level energy, its pressure coefficient and the linear coefficient of its change with Mn molar fraction, namely

$$E_I^{+/0}(p,x)=329\ \text{meV}-102\ \text{meV/GPa}\cdot p$$
$$-1140\ \text{meV}\cdot x\quad \text{for}\ U>0$$

and

$$E_I^{-/+}(p,x)=316\ \text{meV}-93\ \text{meV/GPa}\cdot p$$
$$-1130\ \text{meV}\cdot x\quad \text{for}\ U<0.$$

On the other hand, we find that the problem of the charge state of the iodine impurity center can be experimentally solved by the pressure studies of specially chosen samples. A sample suitable for this purpose should (i)-contain about 20 -25% of Mn (as our sample of $Cd_{0.80}Mn_{0.20}Te:I$) and (ii)-be by far less compensated than the one used in our study.

The presence of the resonant donor level introduces the upper limit of the free-electron concentration in the investigated materials. For CdTe:I this limit is estimated to be about $3\times 10^{19}\ \text{cm}^{-3}$ while for $Cd_{0.80}Mn_{0.20}Te:I$ it is about $5\times 10^{18}\ \text{cm}^{-3}$. For Mn molar fraction $x\approx 0.30$ the impurity level is predicted to enter the forbidden gap.

ACKNOWLEDGMENTS

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APPENDIX

For the positive U model, the concentration of positively charged I centers has the following form

$$N_I^+=\frac{N_I}{1+g\ \exp\left(\dfrac{E_F-E_I}{k_BT}\right)}$$

where g is a degeneracy factor.

For the negative U model the concentration of positively and negatively charged iodine centers have the forms

$$N_I^+=\frac{N_I}{1+g\ \exp\left(\dfrac{2(E_F-E_I^{-/+})}{k_BT}\right)}$$

$$N_I^-=N_I^+g\ \exp\left(\frac{2(E_F-E_I^{-/+})}{k_BT}\right).$$

The above formulas follow from the grand canonical ensemble with the assumption that $|U|\gg k_BT$. The thermal energy $E^{-/+}$ is given per one electron. Since our calculations were performed for a constant temperature $T=190$ K, we have assumed $g=1$, keeping in mind that if $g\neq 1$ the value of E_I would have to be corrected by $k_BT\cdot\ln(g)$ and $0.5k_BT\ln(g)$ for $U>0$ and $U<0$ models, respectively.

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