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TWO-ELECTRON DX STATE IN CdTe:In*

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In this paper we investigate electron emission/capture from/to the DX state of indium in CdTe by means of high pressure freeze-out cycle and steady-state photo-conductivity experiments. The results indicate that the DX state is occupied by two electrons. A comparison with deep level transient spectroscopy data shows that two-electron emission occurs at low temperatures, while one-electron emission takes place at high temperatures.

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It was recently shown that the indium donor state in CdTe exhibits metastable behaviour at low temperatures under hydrostatic pressures (HP) above 7 kbar [1]. It was found that the In related state in CdTe is located 110 meV above the conduction band edge at ambient pressure and has a pressure coefficient of -10 meV/kbar with respect to the conduction band edge [1]. However, the microscopic structure of this center and its charge state are still not experimentally established. In this paper we investigate: (a) electron emission from the DX state under HP after filling this level by a high pressure freeze-out (HPFO) cycle [2]; (b) electron capture on DX under HP in steady-state photoconductivity experiments. The results of our experiments show that the DX state is occupied by two electrons and the barrier for electron emission increases with applied pressure.

We investigate 0.7 μm thick layers of CdTe:In grown by MBE, with the doping level in the range of 5×10^{17}–2×10^{18} cm^{-3} [3].

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In Fig. 1a results of Hall measurements vs. temperature for pressures 0, 3.2 and 5.8 kbar are presented. The electron concentration at 77 K is obtained in HPFO cycle, i.e., at 300 K the pressure $p = 13.5$ kbar was applied, the sample was then cooled down to 77 K, and the pressure was released to the value of 0, 1.5, 3.2, and 5.8 kbar, respectively. After achieving non-equilibrium occupancy of the DX

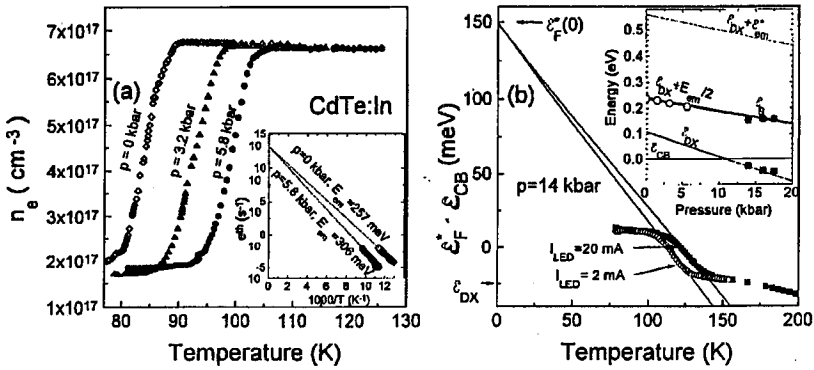

Fig. 1. (a) Electron concentration as a function of temperature after HPFO cycle for pressures of 0 kbar (diamonds), 3.2 kbar (triangles) and 5.8 kbar (dots), respectively. Inset shows Arrhenius plot of the emission rate for 0 kbar (diamonds) and 5.8 kbar (dots). Lines — extrapolation of the experimental results. (b) Quasi Fermi-level position vs. temperature obtained from Hall concentration in steady-state photoconductivity experiments at 14 kbar for different IR LED currents (dots and circles). Lines present extrapolation of the linear slope to $T = 0$ K. Inset shows the pressure dependence of: (i) the positions of the DX state $\mathcal{E}_{DX}$ are shown by the solid line — results obtained in the pressure range up to 14 kbar [1], while the results deduced from the position of the Fermi level for $T = 150$ K from steady-state photoconductivity are shown with squares; (ii) the position of the barrier top for the two-electron process: circles are taken from the emission experiments while dots from steady-state photoconductivity data; the solid line connecting these points is a guide for the eye; (iii) the position of the barrier for one-electron process observed in DLTS experiments at high temperatures — dotted line, where value and pressure dependence of $\mathcal{E}^*_{em}$ were taken from [6].

state at 77 K, the sample was heated with a constant rate of 1 K/min. Characteristic steps in the Hall concentration, $n_e(T)$, observed in Fig. 1a relate to thermally activated emission from the DX state. In the inset of Fig. 1a the Arrhenius plot for the emission coefficient, e^{th}, at different pressures is presented. The analysis of these results, under the assumption that $e^{th}(T) = e^{\infty}_{th} \exp(E_{em}/kT)$†, allowed us to determine the energy barrier for emission, E_{em} : $E_{em}(p) = 255$ meV$+p8.4$ meV/kbar and $e^{\infty}_{th} = 10^{13}$ s^{-1}.

In order to evaluate the position of the barrier top for electron capture, $\mathcal{E}_B$, the photoconductivity in the temperature range 77–300 K under HP up to

†It is well experimentally established that for two-electron emission, the emission rate is defined without factor T^2 before exponent (e.g. see Ref. [4]).

20 kbar was investigated. During Hall effect and conductivity measurements the sample was illuminated (with controlled intensity) by an infrared light-emitting diode (IR LED) incorporated in the pressure cell. Results for $p = 14$ kbar and for different illumination intensities are presented in Fig. 1b. For temperatures higher than 140 K, when the barrier for electron capture/emission to/from DX state is transparent, quasi-Fermi level, $\mathcal{E}_F^*$, is pinned to the DX level position, $\mathcal{E}_{DX}$. (In this paper we denote the one-electron energy by $\mathcal{E}$, and the two-electron energy by $\mathcal{E}$.) The pressure dependence of $\mathcal{E}_{DX}$ is shown by squares in the inset of Fig. 1b.

For 100 K $< T <$ 140 K $\mathcal{E}_F^*$ is defined by the balance between electron thermal capture on the DX state and electron optical emission from DX (below 100 K $\mathcal{E}_F^*$ saturates because of the limited number of donors which are the source of electrons in this system). As it was presented in [4], at steady-state photoconductivity conditions $\mathcal{E}_F^*$ is a linear function of temperature and depends on the illumination of the sample. Extrapolation of $\mathcal{E}_F^*(T)$ to $T = 0$ K allows to estimate the position of the barrier top $\mathcal{E}_F^*(0) = \mathcal{E}_B$. For $p = 14$ kbar, $\mathcal{E}_B$ is about 150 meV above the conduction band edge. Depending on the charge state of the DX level, E_B is equal to $\mathcal{E}_B$ or $2\mathcal{E}_B$ for one- or two-electron states, respectively [4]. On the other hand, $E_B = E_{DX} + E_{em}$, where E_{em} is the activation energy for the emission process (with 1 or 2 electrons). Results of our experiments presented in the inset of Fig. 1b show that the latter equation can be fulfilled only assuming that the DX state captures 2 electrons. The emission process, characterised by the activation energy $E_{em} \approx 250$ meV, corresponds to simultaneous emission of two electrons: $DX^- + 250\ meV \rightarrow 2e + D^+$, i.e., the emission energy per one electron is $\mathcal{E}_{em} = E_{em}/2$.

DLTS experiments performed on CdTe:In samples reveal two emission barriers [5]. The barrier governing the emission for temperatures below 200 K is characterised by low emission rate ($e_{th}^{\infty} \approx 10^{13}$) and is similar to the one observed in our experiments. At temperatures above 240 K, the emission barrier is equal to 450 meV and the emission rate becomes orders of magnitude higher. Since there is no crossing of DLTS lines these two processes are attributed to emission from the same initial state [5]. This result suggests that (1) at low temperature two-electron process takes place and (2) for $T >$ 240 K one-electron transition from the DX state to the one-electron excited state, D_0^*, dominates ($DX^- + 450\ meV \rightarrow e + D_0^*$) with subsequent thermalization of this state.

In conclusion, we have shown that: (a) the metastability of the In donor in CdTe originates from strong lattice relaxation connected with the formation of the negatively charged DX centre; (b) the emission barrier depends on hydrostatic pressure. A comparison of our results with DLTS measurements indicates two different emission paths from the In DX state in CdTe with transfer of one or two electrons.

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