Proc. 25th Int. Conf. Phys. Semicond. (ICPS 25), Osaka (2000), Springer-Verlag Berlin, 1439

Defect-Induced Bound-Exciton Lines in Hydrogen-Doped CdTe: Zeeman Spectroscopy

J. Hamann[1], L. Worschech[2], S. Lany[1], W. Ossau[2], V. Ostheimer[1], C. Schmitz[1], H. Wolf[1], and Th. Wichert[1]

[1]Technische Physik, Universität des Saarlandes, D-66123 Saarbrücken, Germany; e-mail: thw@tech-phys.uni-sb.de
[2]Physikalisches Institut, Universität Würzburg, D-97074 Würzburg, Germany

Abstract More than 50 photoluminescence (PL) lines in the range between 1.591 and about 1.45 eV are observed in nominally undoped CdTe crystals that were treated in a hydrogen plasma at 160 °C. Six of these lines are accessible to a detailed magneto-optical investigation: three lines reveal <111> symmetries, two lines <110> symmetries, and one line a symmetry near the <552> directions. All lines show a strong, uniaxial tensile strain along the symmetry axis, and some of them an electron-hole exchange interaction. The more than 50 lines are caused by the recombination of excitons bound to isoelectronic defects or ionised donors which are formed by at least two constituents being located at different distances and directions relative to one another. At least one of the constituents is a small atom or a vacancy replacing a Cd atom, and hydrogen atoms are probably part of the defects.

Seven new photoluminescence (PL) lines H1-H7 are observable in the excitonic region if nominally undoped, Bridgman-grown CdTe is exposed to a hydrogen plasma at 0.7 mbar and 160 °C for 1 h [1, 2]. Since these lines are also visible after implantation of H^+ ions into CdTe with low energy (200 eV), it is concluded that they are caused by hydrogen-related defects [1, 2]. In spite of the low intensities of these lines, a preliminary investigation of line H3 in a magnetic field was performed in order to get information about the electronic properties and the structure of the corresponding defect [3].

The lines can be produced with much higher intensities by annealing the crystals in vacuum or in a Te atmosphere at moderate temperatures around 600-700 K before the treatment in a hydrogen plasma. Not only seven, but more than 50 new PL lines (called H lines), spread over the energy range between 1,591 and about 1,45 eV, are visible following this treatment. The high energy part of this spectrum, exhibiting the lines H1-H27, is shown in Fig. 1. Since these lines always occur together, all of them are supposed to have a common origin and, consequently, to be hydrogen-related.

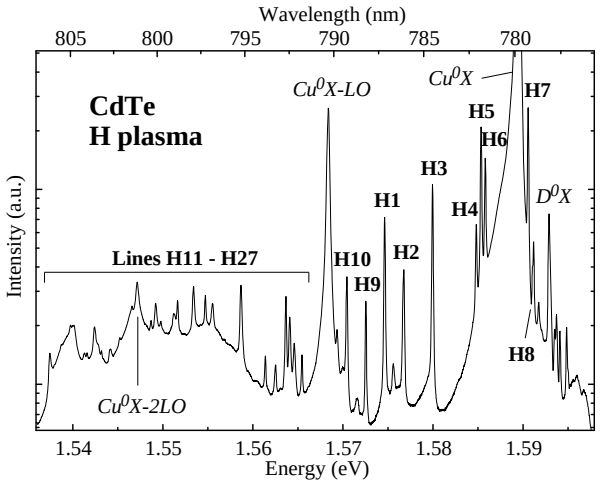

Fig. 1 High energy part of the PL spectrum of a CdTe crystal that has been treated in a hydrogen plasma.

In this contribution, the results of new magneto-optical investigations of the lines H1, H3, H4, H5, H9, and H10 are presented, which partly correct the preliminary conclusions drawn in ref. [3]. In particular, line H9 is discussed in more detail. The peak positions of this line, which were measured at 1.7 K, are shown in Fig. 2. Based on the observed dependence on the strength and the orientation of the magnetic field, the following conclusions are drawn:

(a) The Zeeman splitting pattern obtained by rotating the magnetic field in a (1 1 0) plane can only be explained if the quantisation axes of the angular momenta J = 3/2 of the holes are along the <111> directions of the zincblende lattice. In this simple case, the anisotropy of the Zeeman splitting is mainly a consequence of the changing angles between the four <111> directions and the rotating magnetic field. Hence, the observed defect has a <111> symmetry.

(b) Only the heavy-hole ($J_z = \pm 3/2$) lines are observed. This is concluded because light-hole lines ($J_z = \pm 1/2$) would produce a very different splitting pattern (see e.g. [4]). The light-hole lines are shifted by several meV to higher energies due to the strong, uniaxial tensile strain produced by the defects along their symmetry axes and are

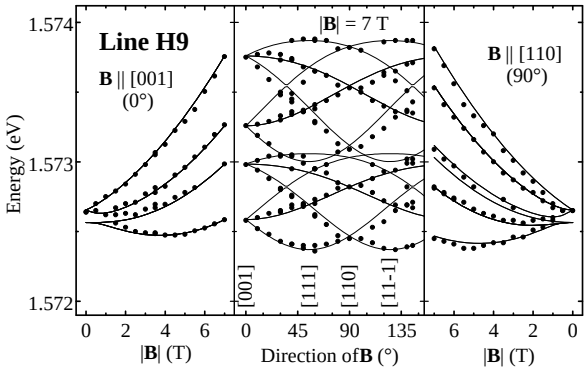

Fig. 2 Peak positions of line H9 in a magnetic field. Left: Variation of |**B**| with **B** || [001] (0°) in Faraday configuration (**k** || **B**). Right: Variation of |**B**| with **B** || [110] (90°) in Voigt configuration (**k** ⊥ **B**). Middle: Dependence on the angle between the [001] direction of the CdTe lattice and the direction of **B** if rotated in the (1 $\bar{1}$ 0) plane at |**B**| = 7 T. The solid lines represent the fit according to the Hamiltonian (1) with the parameters listed in Table 1.

not populated due to thermalisation with the heavy-hole lines.

(c) The Zeeman splitting pattern observed at $|\mathbf{B}| = 7$ T can be divided into two regions: In the lower half all components are connected with the two lower components at $\mathbf{B} \parallel [001]$ and in the upper half with the two upper components at $\mathbf{B} \parallel [001]$. The lower half, which corresponds to the electron spin component $s_z = +1/2$, ($z \parallel \mathbf{B}$), is spread over a smaller energy range than the upper half, which is connected with $s_z = -1/2$. This asymmetry requires an electron-hole exchange interaction. Hence, there is *one* electron and *one* hole in the initial state of the recombination process. (If there were two electrons, their angular momenta would couple to a total angular momentum of zero due to the Pauli principle, thereby preventing an electron-hole exchange interaction. A similar argument would hold for two holes.) Furthermore, the wave functions of the electron and the hole have a large overlap. Therefore, line H9 is caused by the recombination of a bound exciton and not by a donor-acceptor-pair or free-to-bound transition. This conclusion is confirmed by the dependence of the intensities of the H lines (measured without magnetic field) on the excitation power, because it is very similar as for other excitonic lines in the PL spectrum. Since no additional charge carrier is present at the defect, the exciton is bound to an isoelectronic defect or to an ionised donor. (Within the effective-mass theory, excitons bound to ionised acceptors are not stable in CdTe [5].) The exchange interaction also causes the splitting into two lines at $|\mathbf{B}| = 0$ T (see Fig. 2). The lower component cannot be observed, however, because the corresponding transition is dipole forbidden at $|\mathbf{B}| = 0$ T.

The peak positions in Fig. 2 have been fitted by the Hamiltonian

$$H = H_{EX} + H_{LB} + H_{QB} + H_S \qquad (1)$$

which is described in detail in ref. [6]. H_{EX} is the electron-hole exchange interaction; H_{LB} and H_{QB} describe the contributions due to the interaction of the electron and hole angular momenta with the magnetic field and are proportional to $|\mathbf{B}|$ and to $|\mathbf{B}|^2$, respectively (see also [7]). And, H_S describes the influence of the uniaxial strain caused by the defects on the hole angular momentum. The best fit to the peak positions yields the parameters listed in Table 1.

Besides line H9, the lines H1, H3, H4, H5, and H10 yield the following information:

(a) Lines H4 and H5 reveal <111> symmetries, too; lines H1 and H10 are caused by defects with <110> symmetries; and the splitting of line H3 can only be accounted for by uniaxial strains near the <552> directions. The different symmetries are not surprising, because both, the absence of thermalisation between the different H lines and the impossibility of exciting a particular H line by resonant excitation of a different H line, show that each H line is caused by a different defect.

(b) All investigated H lines reveal a strong, uniaxial tensile strain.

(c) The electron-hole exchange interaction is very small for the lines H1, H3, and H5 being a = 0.02(3) - 0.03(3) and is not detectable for line H10. For line H4, this parameter cannot be determined.

(d) The isotropic g-factors (g_e and K in Table 1) are similar for all lines, being in the range between -1.63 and -1.78 for the electrons and between 0.63 and 0.70 for the holes. These values are typical for defects in CdTe [8].

Both, the fact that each defect possesses a symmetry lower than tetrahedral and that more than 50 lines are visible, indicate that at least two constituents form the observed defects. Apart from the different symmetries, the spectroscopic properties of all H lines are very similar. In some cases even the intensities of all lines increase with exactly the same time constant upon illumination by a laser. Therefore, it is concluded that the same constituents form all the observed defects, being located, however, at different distances and directions relative to each other. The tensile strain indicates that at least one of the constituents is a small atom or a vacancy replacing a host atom. A defect consisting exclusively of interstitial and/or large atoms would cause a compressive strain. From the annealing experiments mentioned above, it is concluded that the replaced host atom is a Cd atom. Moreover, hydrogen atoms are probably part of the defects. Since the defects are formed by at least two constituents, probably involving intrinsic defects, and no isotope shift is observed after replacing hydrogen by deuterium [2], it has not been possible to establish the exact identity of the family of defects causing the H lines.

Table 1 The parameters describing the Zeeman effect of line H9 (see ref. [6] for detailed explanations).

g-factors			e-h exchange	
g_e	K	L	a (meV)	b (meV)
-1.78(5)	0.64(3)	0	0.06(3)	0

quadratic Zeeman effect			defect-induced strain	
c_1 (μeV/T^2)	c_2 (μeV/T^2)	c_3 (μeV/T^2)	direction	D (meV)
11.0(5)	0(5)	-1.5(5)	<111>	>1

References

1. J. Hamann, D. Blaß, C. Casimir, T. Filz, V. Ostheimer, C. Schmitz, H. Wolf, Th. Wichert, A. Burchard, M. Deicher, R. Magerle; Appl. Phys. Lett. **72** (1998) 554.
2. J. Hamann, D. Blaß, A. Burchard, C. Casimir, M. Deicher, T. Filz, R. Magerle, V. Ostheimer, C. Schmitz, H. Wolf, Th. Wichert; J. Cryst. Growth **184/185** (1998) 1147.
3. J. Hamann, L. Worschech, D. Blaß, C.Y. Hu, T. Filz, W. Ossau, V. Ostheimer, C. Schmitz, H. Wolf, Th. Wichert; Phys. Stat. Solidi (b) **210** (1998) 513.
4. W.M. Chen, Q.X. Zhao, B. Monemar, H.P. Gislason, P.O. Holtz; Phys. Rev. B **35** (1987) 5722.
5. P.J. Dean, D.C. Herbert; *Excitons*, edited by K. Cho (Springer-Verlag, Berlin 1979) p. 70.
6. L. Worschech, W. Ossau, G. Landwehr; Phys. Rev. B **52** (1995) 13965.
7. K. Cho, S. Suga, W. Dreybrodt, F. Willmann; Phys. Rev. B **11** (1975) 1512.
8. E. Molva, Le Si Dang; Phys. Rev. B **32** (1985) 1156.