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Magneto-Optical Properties of a Hydrogen-Related Defect in CdTe

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Nominally undoped CdTe was exposed to a hydrogen plasma at 160 °C. It has been shown that after this treatment, seven typical photoluminescence lines H_1 to H_7 are observed in the excitonic region. The dependence of the most intense of these hydrogen-related lines, H_3, on external magnetic fields up to $|\mathbf{B}| = 7$ T is investigated. The diamagnetic shift of the H_3 line is proportional to $|\mathbf{B}|^2$, showing that it is caused by the recombination of excitons. Since an electron–hole interaction is observed, the exciton is either bound to an isoelectronic defect or to an ionised donor. The anisotropy of the Zeeman splitting is explained in terms of a small uniaxial compressive strain in a [100] direction perpendicular to the [001] surface orientation. In contrast, the well-known copper-bound exciton line, used as a reference, reveals uniaxial tensile strain in the same [100] direction. Therefore, the defects associated with the H_3 line either have a [100] symmetry or are incorporated close to [100] oriented extended defects. The electron g-factor is $g_e = -1.50 \pm 0.04$, and the hole parameters are $K = 0.40 \pm 0.05$ and $L = 0.00 \pm 0.04$, describing the isotropic and the anisotropic Zeeman effect, respectively.

Introduction. It has recently been shown that after the exposure of undoped CdTe to a hydrogen plasma at 160 °C, seven new photoluminescence (PL) lines H_1 to H_7 are observed in the energy range between 1.575 and 1.591 eV. Since these lines are also visible after a 200 eV implantation of H^+ ions into CdTe, it was concluded that they are caused by the presence of hydrogen in CdTe [1, 2]. High magnetic fields are a proper tool to investigate the electronic and microscopic structure of the associated defects. Only the H_1, H_2, and H_3 lines, however, are well isolated from each other and from other lines, which is favourable for magneto-optical investigations. In this paper, the results obtained from the H_3 line are presented, because this is the most intense line and thus yields the most reliable data. From the Zeeman splittings of the H_1 and H_2 lines, though not identical, similar conclusions can be drawn as for the H_3 line.

Experimental Procedure. Nominally undoped, Bridgman-grown CdTe crystals were exposed to a hydrogen plasma at 160 °C and 70 Pa for 1 h [1, 2]. The magneto-optical investigations were carried out at 1.7 K. The luminescence, excited by an Ar laser, was dispersed by a grating monochromator with a focal length of 1 m and detected by a

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cooled photomultiplier tube. Magnetic fields up to 7 T were produced by a superconducting split coil magnet. Zeeman spectra were recorded in both Voigt ($\mathbf{B} \perp \mathbf{k}$) and Faraday ($\mathbf{B} \parallel \mathbf{k}$) configurations. In order to analyse the anisotropy of the Zeeman splitting, the sample was rotated in small angular steps with the magnetic field oriented in a $(\bar{1}10)$ plane.

Experimental Results and Discussion. It will be shown that the data obtained from the H_3 line reveal uniaxial stress at the site of the defect associated with this line. Therefore, the well-known recombination of excitons bound to neutral copper acceptors (Cu^0X) [3], which dominate the spectrum, was also studied in a magnetic field as a reference for the strain distribution at the investigated sample position.

Fig. 1 shows the peak positions of the Cu^0X line in a magnetic field. A uniaxial stress is deduced because (i) two lines are observed for $|\mathbf{B}| = 0$, and (ii) the Zeeman splitting is clearly anisotropic. If the two lines for $|\mathbf{B}| = 0$ were caused by two different acceptors, each line would split into at least six components [4], and the Zeeman splitting would be nearly isotropic. The Zeeman splitting is analysed, using an effective spin Hamiltonian [3]

$$\hat{H}_{1/2} = g_e \mu_B \mathbf{S} \cdot \mathbf{B} \tag{1}$$

for the initial bound-exciton state $S = \frac{1}{2}$ and

$$\hat{H}_{3/2} = \mu_B [K \mathbf{J} \cdot \mathbf{B} + L(J_x^3 B_x + J_y^3 B_y + J_z^3 B_z)] \tag{2}$$

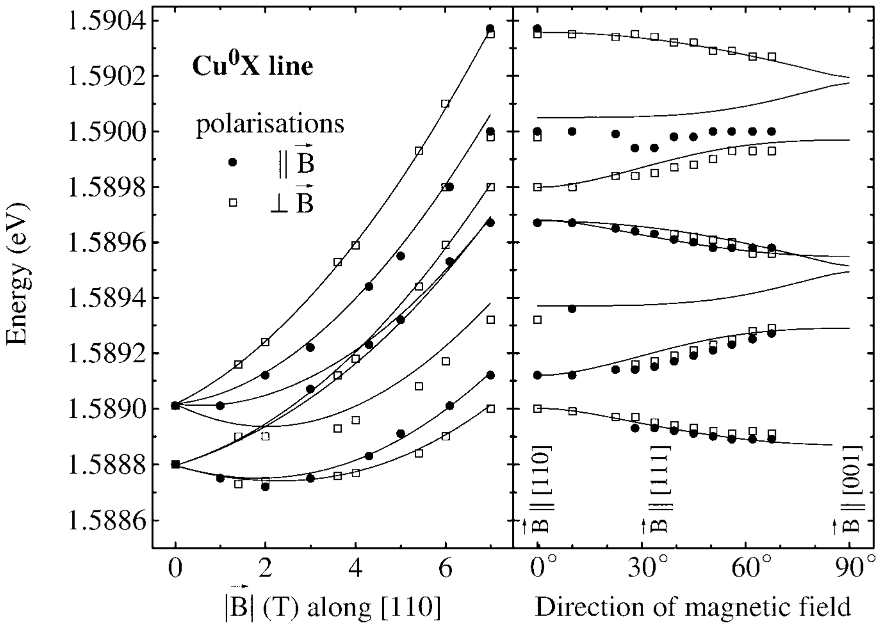

Fig. 1. Peak positions of the Cu^0X line in Voigt configuration with the polarisations $\parallel \mathbf{B}$ and $\perp \mathbf{B}$. Left part: Variation of $|\mathbf{B}|$ with $\mathbf{B} \parallel [110]$. Right part: Angular dependence at $|\mathbf{B}| = 7$ T. The angle between the [110] crystal direction and the magnetic field $\mathbf{B}$ is shown. The lines represent a fit which is explained in the text

for the final acceptor state $J = \frac{3}{2}$ in cubic symmetry, where μ_B is the Bohr magneton, g_e is the electron g-factor, K and L are the hole parameters describing the isotropic and the anisotropic Zeeman effect, respectively.

The diamagnetic shift of an exciton recombination is well described by [4, 5]

$$\hat{H}_{\text{diam}} = c\,|\mathbf{B}|^2\,, \tag{3}$$

where c is the diamagnetic shift parameter of the center of gravity. The influence of uniaxial stress is taken into account by [6, 7]

$$\hat{H}_S = -D[J_\xi^2 - \tfrac{1}{3}\,J(J+1)]\,, \tag{4}$$

where D is the deformation potential and $J_\xi = (lJ_x + mJ_y + nJ_z)$ is the component of the angular momentum $\mathbf{J}$ in the direction of the uniaxial stress. Thus, the Hamiltonian used is

$$\hat{H} = \hat{H}_{1/2} + \hat{H}_{3/2} + \hat{H}_{\text{diam}} + \hat{H}_S\,. \tag{5}$$

The best fit to the data has been obtained with the following parameter values:

$g_e = -1.68 \pm 0.02$, $K = 0.58 \pm 0.04$, $L = -0.02 \pm 0.02$,

$D = (0.10 \pm 0.02)$ meV, $c = (1.50 \pm 0.04) \times 10^{-2}$ meV/T^2.

They are in good agreement with the parameters found in unstrained ($D = 0$) CdTe [3]:

$g_e = -1.77 \pm 0.02$, $K = 0.61 \pm 0.04$, $L = -0.04 \pm 0.02$,

$c = 1.47 \times 10^{-2}$ meV/T^2.

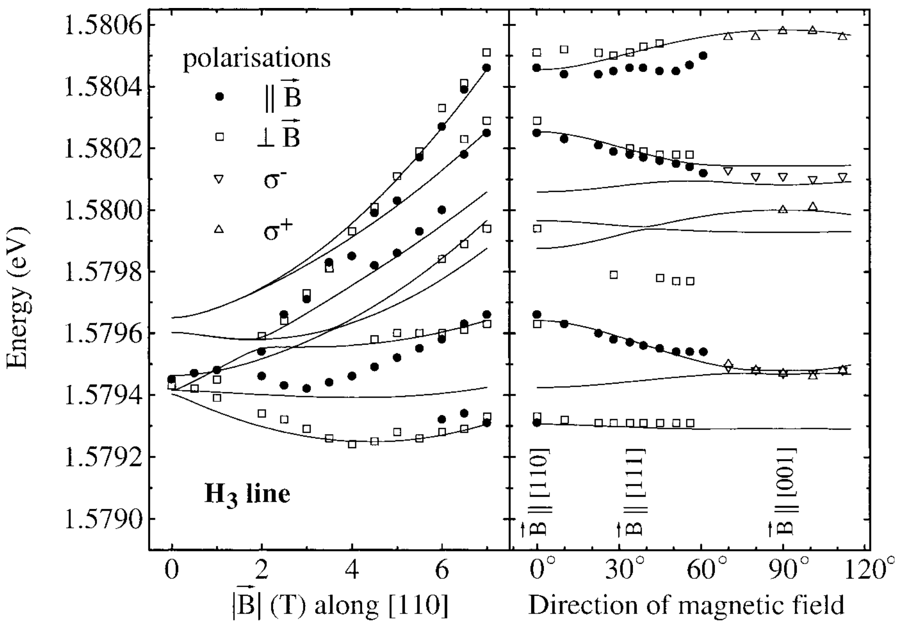

Fig. 2. Peak positions of the H_3 line in Voigt configuration (polarisations $\|\mathbf{B}$ and $\perp\mathbf{B}$) and in Faraday configuration (polarisations σ^- and σ^+). See also Fig. 1

The observed uniaxial stress is tensile, because the Zeeman splitting in Fig. 1 shows that the heavy-hole component ($m_J = \pm\frac{3}{2}$) is lower in energy than the light-hole component ($m_J = \pm\frac{1}{2}$). Its orientation is in a [100] direction perpendicular to the [001] surface orientation. Since the copper acceptor itself has cubic symmetry, the non-zero value of the deformation potential D reflects a global uniaxial strain at the investigated sample position. It should be noted that the center of gravity for $|\mathbf{B}| = 0$ is shifted from the position in unstrained CdTe at 1.5896 eV [8] towards lower energy, probably by hydrostatic strain.

This uniaxial stress is compared with the uniaxial stress observed in the analysis of the anisotropy of the Zeeman splitting of the H_3 line, which is shown in Fig. 2. PL spectra for $|\mathbf{B}| = 0$ and $|\mathbf{B}| = 7$ T are shown in Fig. 3. The interpretation of the Zeeman splitting of the H_3 line is difficult, because it seems to reveal a new kind of defect and the magnetic subcomponents are not very well resolved, whereby the full width at half maximum at $|\mathbf{B}| = 0$ is about 0.28 meV. Nevertheless, several conclusions can be drawn:

a) The diamagnetic shift of the center of gravity of the magnetic subcomponents towards higher energy is proportional to $|\mathbf{B}|^2$. This shows that the H_3 line is caused by the recombination of excitons, because transitions involving conduction band electrons or valence band holes exhibit a linear shift [9]. In addition, as none of the magnetic subcomponents shift to lower energies for $|\mathbf{B}| > 4$ T, two hole transitions and two electron transitions can also be excluded [10].

b) An electron–hole interaction is reflected by the asymmetrical splitting of the four magnetic subcomponents observed in Faraday configuration with $\mathbf{B} \parallel [001]$, i.e. the energetic distances between the two higher components and between the two lower components are not equal. Hence, the exciton cannot be bound to a neutral acceptor, because in the initial state of the acceptor-bound exciton the angular momenta J_1 and J_2 of the two holes would be coupled to $J_1 + J_2 = 0$, which would make an interaction with the electron spin impossible, and in the final state there would be no electron. A coupling to $J_1 + J_2 = 2$ produces a completely different splitting pattern [4]. Similarly, an exciton bound to a neutral donor can be excluded. As an exciton bound to an ionised acceptor is not stable in CdTe [11], the exciton is either bound to an isoelectronic defect or to an ionised donor.

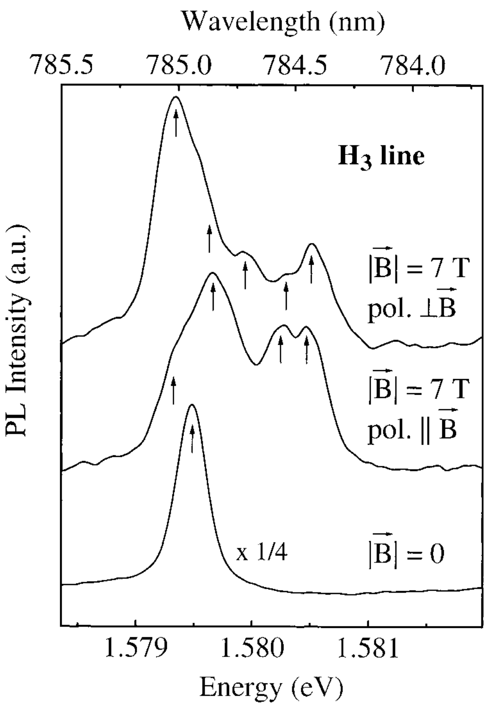

Fig. 3. PL spectra of the H_3 line in Voigt configuration with $\mathbf{B} \parallel [110]$. The arrows indicate the respective peak positions shown in Fig. 2

c) The Zeeman splitting is anisotropic, which indicates uniaxial stress at the position of the defects causing the H_3 line. Since uniaxial stress produces a mixing of the heavy and light hole states, this also explains the fact that the transitions are not completely polarised. A splitting of the H_3 line into two components at $|\mathbf{B}| = 0$, however, is not observed. This can be explained by the observed electron–hole interaction, which for small magnetic fields couples the angular momenta of the electron and the hole to the total angular momentum of the exciton $F = S + J = 1$ or 2, and the transition of the $F = 2$ state into the ground state ($F = 0$) is dipole forbidden.

For the quantitative analysis of the Zeeman data of the H_3 line, the electron–hole interaction

$$\hat{H}_{\text{e-h}} = -a\mathbf{J} \cdot \mathbf{S}\,, \tag{6}$$

with a being a parameter which defines the strength of the electron–hole interaction, was added to the Hamiltonian described by equation (5); $S = \frac{1}{2}$ is the electron spin and $J = \frac{3}{2}$ is the angular momentum of the hole.

The best fit to the data has been obtained with the following parameter values:

$$g_e = -1.50 \pm 0.04, \qquad K = 0.40 \pm 0.05, \qquad L = 0.00 \pm 0.04,$$

$$D = (-0.08 \pm 0.02)\ \text{meV}, \qquad a = (-0.03 \pm 0.02)\ \text{meV},$$

$$c = (7.1 \pm 1)10^{-3}\ \text{meV/T}^2.$$

Additionally, the diamagnetic shift is different for heavy holes and for light holes, which has been observed similarly for the exciton bound to the gold acceptor in CdTe [12]. The fit shown in Fig. 3 well describes the angular dependence of the Zeeman splitting. The absolute values of g_e, K, and c are significantly smaller than the values usually determined for defects in CdTe [3, 4]. These observations suggest a model of strongly localised excitons, because a strong localisation is expected to reduce the values of g_e, K, L, and c [13]. From the sign of the deformation potential D, the uniaxial stress is unequivocally identified to be compressive, while its orientation is in the same [100] direction as the tensile strain of the Cu^0X line. This means that the uniaxial stress at the position of the defects causing the H_3 line is not the same as in the rest of the sample which is represented by the copper acceptors. There are two possible explanations for this observation. Either the defects have a [100] symmetry themselves, thereby causing the local strain, and are all aligned along the same [100] direction, due to the strained environment. Or the defects are incorporated close to [100] oriented extended defects, which locally induce uniaxial compressive strain.

In conclusion, the H_3 line is caused by the recombination of strongly localised excitons, because the diamagnetic shift of the H_3 line is proportional to $|\mathbf{B}|^2$, and the absolute values of g_e, K, and c are smaller than the values usually determined for defects in CdTe. Since an electron–hole interaction is observed, the excitons are either bound to isoelectronic defects or to ionised donors. The defects associated with the H_3 line either have a [100] symmetry or are incorporated close to [100] oriented extended defects.

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