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Localization of Y Luminescence at Glide Dislocations in Cadmium Telluride

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Abstract. — We demonstrate unambiguously that the well-known defect-related Y luminescence band at 1.476 eV in CdTe originates from the polar Te(g) glide dislocation segments. Crystallographically defined glide dislocation arrangements produced by local plastic deformation on $(\bar{1}\bar{1}\bar{1})$ Te surfaces using Vickers microindentation were characterized by temperature-dependent cathodoluminescence (CL) microscopy as well as CL and PL spectroscopy. The identification of the Te(g) dislocation was obtained by determining the surface polarity applying X-ray diffraction and subsequently revealing the volume glide geometry observed by CL imaging after stepwise depth-etching of the ($\bar{1}\bar{1}\bar{1}$) sample surface. From the spectral and recombination-kinetic properties of the dislocation-bound Y luminescence the model of radiative decay of dislocation-related excitons is supported. Particularly, we may conclude that they are bound to energy levels in the fundamental gap localized at the 90° Te(g) partial dislocations

1. Introduction

In CdTe, among other II-VI compound semiconductor materials, the so-called Y luminescence band has often been observed using photoluminescence (PL) and cathodoluminescence (CL) techniques [1–7]. It occurs predominantly in heteroepitaxial layers made by Molecular Beam Epitaxy (MBE) or Metal Organic Chemical Vapour Deposition (MOCVD) containing interfaces to the GaAs or InSb substrates used. These layers – with thicknesses larger than the critical value of about 1 μ m – exhibit a significant lattice misfit, so that a general correlation of the Y emission intensity with extended defects, for example described by the etch pit density [6], could be demonstrated.

This Y band is characterized by a zero-phonon line at $E_0 = 1.474$ to 1.476 eV measured at temperatures between 2 and 11 K having a rather large linewidth of 8 to 9 meV as well as an anomalously weak LO phonon coupling with a Huang-Rhys factor S = 0.16 to 0.4.

From these observations which are unusual for such a "deep level" emission, Dean [8] developed the model of a special recombination mechanism characterized by deeply defect bound excitons (BE) which are bound in the delocalized potential of a small extended defect such as

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a dislocation loop. This model may well explain the lineshape and phonon coupling properties found. Up to now, however, the Y luminescence has been confirmed only on grown-in defect configurations in CdTe. A definite proof for the relation to a specific defect, in particular, to fresh glide dislocations has not been established yet. Only for a related feature in ZnSe a connection with glide dislocations has been reported [9].

In this paper, we investigate the Y luminescence by means of high resolution, temperature dependent CL experiments in the SEM (Scanning Electron Microscope) after local plastic deformation of CdTe bulk crystals, thereby producing a defined polar glide dislocation arrangement [10,11]. The unambiguous identification of the Y luminescence band as originating from 60° Te(g) dislocation segments will be demonstrated.

2. Experimental Details

The CL and PL studies have been performed on nominally undoped (111) CdTe single crystals grown by a modified Bridgman method From the low temperature PL spectra, the samples revealed to be p-type with a carrier concentration in the range (1 to 5) $\times 10^{15}$ cm⁻³. The sample surfaces were chemo-mechanically polished using 1% bromine in methanol solution. A well-calibrated stepwise removal of surface layers was obtained using the same etchant. The polarity of the ±(111) surfaces was determined by X-ray diffraction [12].

Plastic microdeformation was carried out by indenting the $(\bar{1}\bar{1}\bar{1})$ Te surface with a Vickers diamond pyramid at room temperature. The load was 0.05 to 0.4 N with a dwell time of 15 s.

The deformed samples were examined by means of CL microscopy and locally resolved spectroscopy using a modified SEM Tesla BS 300 equipped with a liquid helium stage and a spectral CL system. This allows a variation of the sample temperature from 5 to 300 K as well as spectroscopic investigations in the range from 400 to 1000 nm. PL spectra were recorded using 514 nm Ar⁺ laser excitation with a spot size of 500 μ m at 1.7 K.

3. Results

3.1. CL MICROSCOPY AND SPECTRAL INVESTIGATION OF LOCALIZED LUMINESCENCE DUE TO GLIDE DISLOCATIONS. — Figure 1 shows a panchromatic CL micrograph from the region around an indentation area on the $(\bar{1}\bar{1}\bar{1})$ Te sample surface at 5 K. The identification of the surface polarity is detailed in Section 3.3. The three-fold symmetric dislocation rosette configuration is clearly resolved with distinct bright CL contrasts obviously originating from single glide dislocations in only one of the two parallel branches of each rosette arm whereas the other branch appears to show dark dislocation contrasts.

Local CL spectra were recorded in the region of the bright dislocation contrasts using a scanning area of about 10 μ m × 10 μ m containing a few bright contrasts of single dislocations. The CL spectra at 5 K exhibit an additional, rather broad, asymmetric band which peaks at 1.476 eV, *i.e.* 130 meV below the CdTe band gap at $E_g = 1.606$ eV (Fig. 2). In a recent work [13], we have called this feature Dislocation Luminescence (DL). This DL emission band is found to be fully localized at the bright dislocation branches and is not detected either in the neighbouring dark contrast branch or in the undeformed matrix area. In the latter regions, the spectrum shows only the bound acceptor and free exciton related near-band-gap emission around 1.595 eV. On the other hand, the matrix band is remarkably reduced in the DL sites. In order to keep the beam excitation power low and to prevent possible degradation effects, a rather large spectrometer slit width was used during the SEM investigations at the single dislocations resulting in a limited spectral resolution of the CL bands. However, by performing





Fig. 1. — a) Panchromatic CL image of an indented $(\bar{1}\bar{1}\bar{1})$ Te surface of CdTe at 5 K (beam voltage 20 kV, beam current 1 nA) illustrating a dislocation rosette with three-fold symmetry. b) CL bright contrasts are localized at one type of the polar dislocation branches of each rosette arm whereas the other branch exhibits dark contrasts.



Fig. 2. — Micro-CL spectra at 5 K (beam voltage 20 kV, beam current 1 nA) from the $(\overline{1}\overline{1}\overline{1})$ Te surface of CdTe recorded at Te(g) dislocations (solid line) as well as in the undeformed matrix region (dashed line). The PL spectrum measured on the same sample at 1.7 K is also shown together with a fitted simulation consisting of the 1.476 eV Y band and another band at 1.448 eV.

PL measurements on the same sample, the DL band feature could be better resolved. From the DL lineshape with its main peak at 1.476 eV followed by several phonon replicas rapidly decreasing in amplitude towards lower energy, the spectral structure could be clearly identified as the well-known Y luminescence in CdTe. A quantitative lineshape analysis using

$$I_{\rm PL}(h\nu) = A \sum_{k=0}^{\infty} e^{-S} \frac{S^k}{k!} \frac{1}{1 + (h\nu - E_0 + kE_{\rm LO})^2 / \Gamma^2}$$
(1)

where k is the number of emitted LO phonons of energy $E_{\rm LO} = 21.3 \text{ meV} [1]$, yields the zerophonon line position $E_0 = (1.476 \pm 0.001) \text{ eV}$, a lineshape broadening of $\Gamma = (10 \pm 2) \text{ meV}$ and a Huang-Rhys factor $S = (0.22 \pm 0.05)$ in very good agreement with the literature value S = 0.2 [1]. An underlying second transition series with zero-phonon peak at about 1.448 eV (S = 2.0) was added to the simulated lineshape. It may be tentatively assigned as caused by (D_0, A_0) donor-acceptor pair recombination involving neutral Cu acceptors as found in reference [14].

3.2. TEMPERATURE DEPENDENCE OF THE DISLOCATION-RELATED Y LUMINESCENCE. — The temperature dependence of the glide dislocation related Y luminescence has been studied in order to explore its recombination-kinetic nature. First, it has been found that the Y band peak position moves to lower photon energies with increasing temperature. This shift proceeds fully parallel to the temperature dependent fundamental gap energy shift $E_g(T)$, whereby a constant optical binding energy of 130 meV is obtained [13]. Secondly, it is known from previous investigations [13] that the dislocation luminescence is rapidly quenched above temperatures of approximately 120 K. From this temperature dependence of the Y band intensity, a thermal activation energy E_A for the quenching process could be determined.

The derivation of the thermal activation energy requires a suitable recombination-kinetic analysis of the DL intensity in comparison with the matrix recombination channels. Following the ideas of Dean [8], the Y luminescence is caused by the radiative decay of excitons bound to defect-related extended states. The radiative recombination process is thus governed by the capture of free excitons and the thermal release of the bound excitons from the defect states. The application of the principle of detailed balance results in the following expression for the ratio $V = I_Y/I_0$ of Y and matrix luminescence intensities [15]

$$V(T) = \frac{V_0}{1 + CT^{3/2} \exp(-E_{\rm A}/kT)}.$$
(2)

Here, C is a constant determined by the ratio of exciton thermal reemission and recombination rates and $V_0 = V(T = 0)$. The normalization to $I_0(T)$ eliminates the temperature dependence of the free exciton concentration. The $T^{3/2}$ factor arising from the effective density of exciton states has often been omitted in a simplified analysis which may result in the appearance of two different activation energy values over the investigated temperature range [4,7].

Figure 3 shows corresponding Arrhenius plots of the intensity ratio V(T) as well as of the matrix luminescence $I_0(T)$ both normalized to their maximum values V_0 and $I_0(0)$, respectively, at low temperatures. The whole temperature range up to 300 K for the matrix band and 120 K for the Y luminescence can be sufficiently well fitted by equation (2). The thermal activation energy for the Y luminescence is determined to be $E_A = (11 \pm 1)$ meV. Comparing this figure to the exciton binding energy of 10 meV in CdTe [16], this result strongly supports the bound exciton mechanism. On the other hand, we do not find a second, larger activation energy from the temperature dependence as in [4]. The matrix luminescence has an activation energy of 34 meV in accordance with [17].

To correlate the temperature-dependent behaviour of the Y luminescence with defect-bound emission, we also performed temperature dependent panchromatic CL defect contrast measurements on isolated dislocations (Fig. 4). This gives an activation energy of 13 meV which



Fig. 3. — Temperature dependence of the ratio $I_{\rm Y}(T)/I_0(T)$ between the dislocation-related Y and matrix luminescence intensities as well as of the matrix luminescence intensity $I_0(T)$, both normalized to their maximum values at low temperatures (symbols). The solid lines represent the fitted temperature-dependent recombination statistics.

is very close to the above given value. Although this procedure cannot give the exact value for E_A since the CL defect contrast c is in general the sum of two parts representing radiative and nonradiative defect-related recombination processes [13], it is a sufficient argument to show that the Y luminescence is indeed localized on the single glide dislocations.

3.3. IDENTIFICATION OF THE POLAR DISLOCATION TYPES. — The reliable identification of the type of dislocations in the bright and dark rosette branches is only possible if both the polarity of the surface studied and the geometrical arrangement of polar Cd(g) and Te(g) dislocations after plastic deformation are known. The latter can be deduced by using the scheme of activated glide systems at the indentation rosette on the $(\bar{1}\bar{1}\bar{1})$ Te surface as illustrated in Figure 5 [10]. It determines the expected Cd(g) and Te(g) dislocation distribution as to be displayed in the CL images. As the dislocation glide for local indentation may occur on the various {111} glide planes in the crystal, the surface-parallel so-called rosette or tangential glide processes and the tetrahedral or volume glide mechanisms have to be distinguished. The surface-parallel rosette glide generates dislocation segments propagating on the (111)Cd and $(\bar{1}\bar{1}\bar{1})$ Te slip planes of the glide prisms [18] as represented in the right part of the figure. Therefore, two parallel branches of a dislocation rosette arm containing either Cd(g) or Te(g) type threading dislocations as well as surface-parallel screw dislocation segments are formed along the surface-parallel $\langle 110 \rangle$ directions.

On the other hand, the tetrahedral or volume glide proceeds with Burgers vectors $\mathbf{b} = a/2\langle 101 \rangle$ inclined to the surface being represented by triangle dislocation patterns near the indentation centre. For example, on the $(1\bar{1}\bar{1})$ Te surface, the activated $(1\bar{1}\bar{1})$, $(\bar{1}1\bar{1})$, and $(\bar{1}\bar{1}1)$ Cd planes form an external apex tetrahedron (EAT) whereas $(11\bar{1})$, $(1\bar{1}1)$, and $(\bar{1}11)$ Te



Fig. 4. — Temperature dependence of the bright panchromatic CL dislocation contrast $c(T) = [I_D(T) - I_0(T)]/I_0(T)$ and the corresponding intensities $I_D(T)$, $I_0(T)$ measured on an isolated threading Te(g) glide dislocation. The inset shows representative CL intensity linescans of the panchromatic signal and the DL band with maximum values I_D and I_{DL} , respectively, at T = 30 K (beam voltage 20 kV, beam current 1 nA).

planes result in an internal apex tetrahedron (IAT) orientation as shown in the left part of Figure 5.

In order to identify the dislocation types unambiguously, the absolute polarity of the investigated crystal surfaces has been determined by X-ray diffraction using the Warekois convention [12]. From the X-ray structure factors, the intensity ratios of the (111) and (333) Cr K $\alpha_{1,2}$ reflexes between the (111)Cd and $(\bar{1}\bar{1}\bar{1})$ Te surfaces are expected to be $I_{Cd}^{(111)}/I_{Te}^{(111)} = 1.13$ and $I_{Cd}^{(333)}/I_{Te}^{(333)} = 0.88$, respectively [12]. The experimental values for the integrated intensity ratios of non-indented to indented side are 1.17 and 0.83, hence identifying the investigated sample surface with the microindentations as the $(\bar{1}\bar{1}\bar{1})$ Te surface.

By stepwise removal of surface layers of definite thickness the bright rosette branches are observed to be reduced in extension and a bright triangle belonging to the tetrahedral glide appears (Fig. 6). It increases in size with depth, thus verifying an EAT orientation. At an etching depth of 26 μ m below the initial surface, the branches of the rosette glide have disappeared and below 70 μ m no glide dislocation could be observed.

Therefore, the volume glide along the EAT for $(\overline{111})$ Te orientation clearly identifies the bright defect contrasts as related to 60° Te(g) dislocations whereas Cd(g) dislocations and possibly screw segments possess a dark CL contrast.



Fig. 5. — Geometry of the rosette glide system around the microindentation on a (111) surface. Glide dislocation slipping on $(1\bar{1}\bar{1})$, $(\bar{1}1\bar{1})$ and $(\bar{1}\bar{1}1)$ Cd planes are of Te(g) type. In the case of a $(1\bar{1}\bar{1})$ Te surface, these planes have an acute angle to the surface. Cd(g) dislocations glide on $(\bar{1}11)$, $(1\bar{1}1)$ and $(11\bar{1})$ Te planes with an obtuse angle to the surface. The left part represents the internal (IAT) and the external apex tetrahedron (EAT) showing the glide planes for Cd(g) and Te(g) dislocations, respectively, on the $(1\bar{1}\bar{1})$ Te surface, or *vice versa* on the (111)Cd surface

4. Discussion and Conclusions

The performed SEM-CL studies revealed Y luminescence in CdTe after plastic deformation of bulk samples. It has been shown by detailed microscopic and spectroscopic investigations that the defect-related emission at 1.476 eV is clearly localized at single fresh 60° Te(g) glide dislocation segments. The dislocation-bound luminescence has been unambiguously identified as the previously observed Y luminescence band caused by the radiative decay of defect-bound excitons. The small thermal activation energy of $E_{\rm A} = 11$ meV contradicts, however, the dislocation exciton model proposed for the Y luminescence in ZnSe [5].

Since the Y band originates from the Te(g) type glide dislocations but not from the other dislocations in the samples, this emission should have distinct correlation with the polar core structure of the dislocations. Öberg [19] performed theoretical calculations of the electronic structure of glide dislocations in CdTe being dissociated into 30° and 90° partials and predicted for the 90° Te(g) partial dislocation the occurrence of a one-dimensional band located in the band gap above $E_V + 0.1$ eV which is in remarkable agreement with the optical binding energy found. This band located at the Te(g) dislocation core has acceptor character and could give rise to the dominating radiative defect recombination path. Since the low thermal activation energy of 11 meV cannot explain the localization potential of 120 meV alone, it is believed that the hole rather than the electron is more strongly bound to the acceptor state [8]. The thermal quenching process is thus interpreted as the removal of the weaker bound electron from the bound exciton complex, *i.e.* the thermal dissociation of the exciton for which only the small electron-hole exciton binding energy is required.



Fig. 6. — a) Panchromatic CL image of an indented $(\bar{1}\bar{1}\bar{1})$ Te surface after removal of a 6 μ m thick layer b) Panchromatic CL image at an etching depth of 18 μ m The rosette glide contrasts are nearly vanished and the bright triangle increases in luminescence intensity and extension. c) At an etching depth of 26 μ m below the surface only the enlarged bright triangle is visible

Finally, it should be noted that another defect-induced luminescence feature at 1.542 and 1.550 eV, that means 60 meV below $E_{\rm g}$ being different from the one discussed here has been found earlier [20]. Since those samples were prepared by uniaxial plastic deformation, another type of defect is supposed to be responsible for the dislocation emission in [20].

Acknowledgments

N°7

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References

- Dean P.J., Williams G.M. and Blackmore G., Novel type of optical transition observed in MBE grown CdTe, J. Phys. D 17 (1984) 2291-300.
- [2] Choyke W.J., Burke M.G., Feng Z.C., Hanes M.H. and Mascarenhas A., Defect-related luminescence in molecular beam epitaxy grown CdTe films, *Mater. Sci. Forum* 10-12 (1986) 769-774.
- [3] Fujii S., Terada T., Fujita Y. and Iuchi T., New deep-level photoluminescence bands of homoepitaxial CdTe films grown by metalorganic chemical vapor deposition, Jpn J. Appl. Phys. 28 (1989) L 1712-1714.
- [4] Onodera C. and Taguchi T., A new 1.47 eV defect-luminescence band in MOCVD-grown CdTe on (100) GaAs, J. Cryst. Growth 101 (1990) 502-506.
- [5] Rebane Yu. T. and Shreter Yu. G., Dislocation-related excitons in semiconductors, Polycrystalline semiconductors II, J.H. Werner and H.P. Strunk, Eds., Springer Proc. Phys. vol. 54 (Springer-Verlag, Berlin 1991) p. 28-39.
- [6] Seto S., Tanaka A., Takeda F. and Matsuura K., Defect-induced emission band in CdTe, J. Cryst. Growth 138 (1994) 346-351.
- [7] Brink D.J. and Kunert H.W., Photoluminescence of CdTe thin films containing a mixed crystal orientation, J. Appl. Phys. 78 (1995) 6720-6725.
- [8] Dean P.J., Comparison of MOCVD-grown with conventional II-VI materials parameters for EL thin films, *Phys. Stat. Sol.* (a) 84 (1981) 625-646.
- Batstone J.L., Cathodoluminescence and transmission electron microscopy chracterisation of ZnSe, Thesis (Bristol 1985).
- [10] Leipner H.S., Schreiber J., Uniewski H. and Hildebrandt S., Dislocation luminescence in the compound semiconductor cadmium telluride, to be published in *Scanning Microscopy*.
- [11] Uniewski H., Schreiber J., Hildebrandt S. and Leipner H.S., SEM CL studies on polar glide dislocations in CdTe, *Mater. Sci. Eng. B* 42 (1996) 284-288.
- [12] Warekois E.P., Lavine M.C., Marino A.N. and Gatos H.C., Crystallographic polarity in the II-VI compounds, J. Appl. Phys. 33 (1962) 690-696.
- [13] Schreiber J., Hildebrandt S., Uniewski H. and Bechstein V., Investigation of the lowtemperature CL contrasts of dislocations in compound semiconductors, *Mater. Sci. Eng.* B 42 (1996) 24-31.
- [14] Stadler W., Photolumineszenzuntersuchungen an CdTe-Volumenkristallen, Diploma thesis (München 1991).
- [15] Zimmermann H., Boyn R. and Piel K., Thermal quenching of bound exciton emission due to phonon-induced non-radiative transitions: experimental data for CdTe and InP, J. Phys. C 4 (1992) 859-868.

- [16] Marple D.T.F., Effective electron mass in CdTe, Phys. Rev. 129 (1963) 2466-2470.
- [17] Bryant P.J., Totterdell D.H.J. and Hagston W.E., Evaluation of the nature of the radiative emission processes from lattice defect centres in cadmium telluride together with the associated quenching mechanisms, *Phys. Stat. Sol.* (a) 14 (1972) 579-590.
- [18] Braun C., Helberg H.W. and George A., Surface damage of CdTe produced during sample preparation, and determination of dislocation types near microhardness indentations, *Philos. Mag. A* 53 (1986) 277-284.
- [19] Oberg S., Electronic state calculations of dislocations in cadmium telluride, Phys. Stat. Sol. (b) 108 (1981) 357-362.
- [20] Tarbaev N.I., Shepel'skii G.A. and Schreiber J., Plasticity of cadmium telluride at 77 K observed by luminescence methods, Sov. Phys. Solid State 31 (1989) 1348-1350.