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Electron Diffraction Study of Twinning in Epitaxial CdTe and $Hg_{1-X}Cd_XTe$ Layers

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Structure of thin CdTe and HgCdTe layers obtained by pulse laser deposition has been investigated by transmission electron diffraction method. Diffraction patterns are of twelve-folded axial symmetry, which proves a double positioning twinning. Observed Debye rings were compared with those predicted by theory for the {111} twinnings of [111] textured samples.

Keywords: CdTe, $Hg_{1-x}Cd_xTe$, 3-d defects, electron diffraction, twinning, epitaxial layers.

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I. Introduction

The growth and structure of epitaxial films of II-VI semiconductors was systematically investigated over the last three decades. Nevertheless such studies are still actual due to novel methods of deposition of films (e.g. MBE, MCVD) as well as to the development of electronic industry towards to nanotechnology stage of fabrication of electronic materials (quantum wells, quantum dots etc.).

Holt [1-2] summarized a great number of experimental results on vacuum-evaporated II-VI compounds onto several substrates (Si, Ge, NaCl, mica etc.). A number of Cd and Zn chalcogenides epitaxial films contained three-dimensional defects as twins and included grains of second phase. Transmission electron diffraction was used for detection of these defects basing on the interpretation of satellite diffraction spots generated by twins in evaporated films of gold studied by Pashley and Stowell [3].

We study diffraction patterns of CdTe and HgCdTe (x = 0.2) films obtained by pulsed laser deposition method (PLD) [4]. An interpretation of the diffractions bases on theoretical calculations of Debye rings for twins in these compounds.

II. Experimental

Thin epitaxial layers of CdTe and HgCdTe (x = 0.2) have been obtained by PLD method using YAG:Nd^{3+} laser [4] on (001) cleaved KCl and NaCl substrates. The parameters of layers deposition are collected in Table 1. The layers were separated from the substrate by dissolution in distilled water.

Structure investigations were carried out using high-energy transmission electron diffraction method (THEED). The transmission microscope JEOL JEM-6A (the high-resolution mode) with voltage of 50kV as well as the electron diffractograph EG-100A with voltage of 80 kV were applied. Figures 1 and 2 presents diffraction

Table 1

Technological parameters of layer deposition

Sample number	Layer	Target	Substrate	Substrate temperature	Thickness	Pulse number
1	$Hg_{1-x}Cd_xTe$ (x = 0.2)*	$Hg_{1-x}Cd_xTe$ (x = 0.2)*	KCl	473 K	350 nm	100
2	CdTe	CdTe	KCl	560 K	170 nm	50

patterns for CdTe, and $Hg_{1-x}Cd_xTe$ samples (Table 1), respectively.

III. Twinnings in CdTe and $Hg_{1-x}Cd_xTe$ crystals and electron diffraction

The crystal structure of single CdTe and $Hg_{1-x}Cd_xTe$ crystals is of the sphalerite type. Thin epitaxial layers of these compounds may include also additional phase of the wurtzite type treated as three-dimensional defects. However, in thin layers deposited from vapour phase, the main 3-D defects are formed by twining [5]. In sphalerite structure, likewise as in diamond structure the twinning occurs on {111} planes as a 180° rotation (or reflection) of one part of the crystal (twin) in respect to other one (matrix) [6,7]. Fig. 2 presents twinning in diamond structure formed on (111) plane. In fact, there are four equivalent directions <111> in diamond-type crystals. Therefore, one can observe four orientations of twins formed in the first stage of twining (twins of the first order).

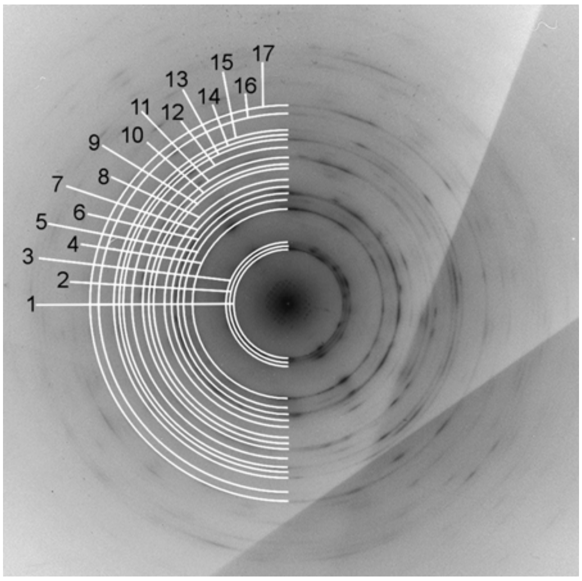

Fig. 1. Transmission electron diffraction pattern of CdTe epitaxial films grown on (001) KCl.

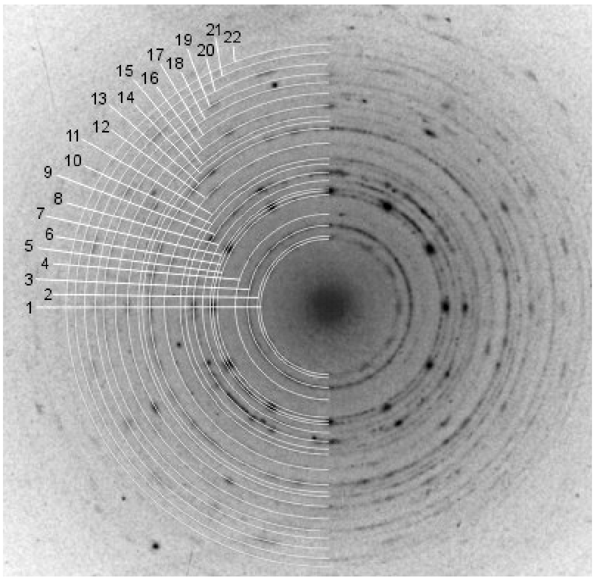

Fig. 2. Transmission electron diffraction pattern of $Hg_{1-x}Cd_xTe$ ($x = 0.2$) epitaxial film grown on (001) KCl.

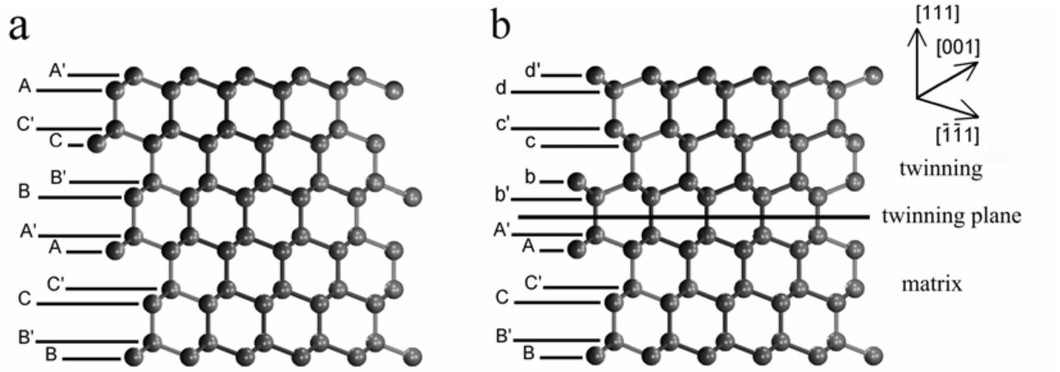

Fig. 3. Diamond crystal structure; a) non-defected, b) twinned.

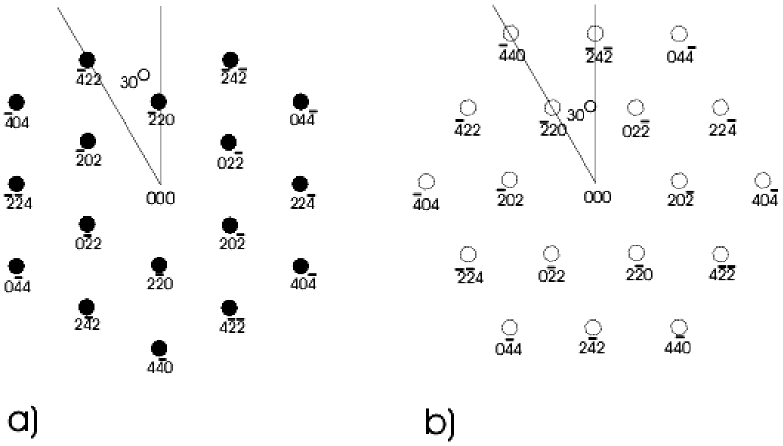

Fig. 4. Diffraction patterns of two positioning nucleons oriented in [111] direction.

Table 3

Comparison of crystallographic spaces (diffraction rings) calculated theoretically with those obtained experimentally for $Hg_{1-x}Cd_xTe$ (a = 6.463 Å) [9] layer

Single $Hg_{1-x}Cd_xTe$ (calculated)		Twinning diffraction		Experiment	
Indexing	Spacing [Å]	Indexing	Spacing [Å]	Nr. of ring	Spacing [Å]
		111^{2-}	5.597		
		111^{-}	3.957		
				1	3.901±0.040
(111)	3.731			2	3.724±0.037
		111^{+}, 200	3.231	3	3.263±0.033
				4	2.844±0.025
		111^{2+}	2.798		
		220^{-}	2.715		
				5	2.374±0.025
(220)	2.285	311^{3-}	2.285	6	2.292±0.023
		220^{+}	2.238	7	2.238±0.022
		311^{2-}	2.115	8	2.098±0.021
		311^{-}	1.978	9	1.965±0.020
(311)	1.948	220^{2+}	1.948		
		222*, 311^{+}	1.865	10	1.855±0.019
		311^{2+}	1.769	11	1.788±0.019
		400^{-}	1.748		
		311^{3+}, 331^{3-}	1.687		
(400)	1.615	331^{2-}	1.615	12	1.619±0.016
		331^{-}	1.495	13	1.483±0.016
(331)	1.482	422^{2-}, 400^{+}	1.482		
		420*, 331^{+}	1.445		
				14	1.427±0.014
		333^{2-}	1.399	15	1.390±0.014
		422^{-}	1.388		
		331^{2+}	1.357		
(422)	1.319	422, 311^{3+}	1.319	16	1.319±0.013
		422^{+}	1.310		
		333^{-}	1.284		
(333)	1.243	422^{2+}, 440^{-}	1.243	17	1.243±0.012
		333^{+}	1.193		
		422^{3+}, 442^{2-}	1.186	18	1.178±0.012
(440)	1.142				
		440^{+}, 422^{-}	1.136	19	1.138±0.011
		333^{2+}	1.119		
		531, 442^{-}	1.092	20	1.090±0.011
(442)	1.070				
		440^{2+}, 442^{+}	1.053	21	1.045±0.011
		442^{2+}	1.017	22	1.012±0.010
		533, 422^{3+}	0.985		

In transmission electron diffraction (TED) the sphalerite and face-centred cubic structure (f.c.c.) have equivalent reciprocal lattices, thus they give the same set of permitted reflections. These two structures are equivalent for TED purposes. This is true also for those twinned structures, where satellite diffraction spots appear around matrix (single crystal) ones. Therefore the analysis of an electron diffraction patterns carried out by Pashley and Stowell [3] for epitaxial f.c.c. metal films can be applied to our semiconductor layers. Twin points (satellite spots) can be considered as [3]:

$$(h'k'l') = (H \pm 1/3u \quad K \pm 1/3v \quad L \pm 1/3w), \qquad (1)$$

where (h’k’l’) is the twin spot obtained from (hkl) matrix spot, (HKL) is the matrix spot and [uvw] is an axis of twining.

In Table 2 and 3 we have calculated all twin crystallographic spaces which arise from satellite spots (eq. 1) for CdTe and $Hg_{1-x}Cd_xTe$ (x = 0.2) crystals, respectively. These spaces are compared with those, which were calculated from Debye rings obtained experimentally (Fig. 1 and 2). The scheme of diffraction

Table 2

Comparison of crystallographic spaces (diffraction rings) calculated theoretically with those obtained experimentally for CdTe (a = 6.481 Å) [8] layer

Single CdTe (calculated)		Twinning diffraction		Experiment	
Indexing	Spacing [Å]	Indexing	Spacing [Å]	Nr. of ring	Spacing [Å]
		111^{2-}	5.612		
		111^{-}	3.968	1	3.986±0.040
(111)	3.741			2	3.720±0.037
				3	3.493±0.035
		200, 111^{+}	3.24		
		111^{2+}	2.806		
		220^{-}	2.722		
(220)	2.291	311^{3-}	2.291	4	2.290±0.023
		220^{+}	2.245		
		311^{2-}	2.121		
				5	2.086±0.021
		311^{-}	1.984		
(311)	1.954	220^{2+}	1.954	6	1.962±0.020
		222*, 311^{+}	1.870	7	1.855±0.018
		311^{2+}	1.774		
		400^{-}	1.753	8	1.753±0.016
		311^{3+}, 331^{3-}	1.692		
(400)	1,620	331^{2-}	1.620	9	1.611±0.016
		331^{-}	1.500		
				10	1.553±0.015
(331)	1.486	422^{2-}, 400^{+}	1.486	11	1.487±0.015
		420*, 331^{+}	1.449		
		333^{2-}	1.403	12	1.395±0.014
		422^{-}	1.392		
		331^{2+}	1.361		
(422)	1.322	311^{3+}	1.322	13	1.324±0.013
		422^{+}	1.313		
		333^{-}	1.287	14	1.286±0.013
(333)	1.247	422^{2+}, 440^{-}	1.247	15	1.247±0.012
		333^{+}	1.196		
		422^{3+}, 442^{2-}	1.189		
(440)	1.145			16	1.146±0.012
		440^{+}, 422^{-}	1.139		
		333^{2+}	1.122		
		531, 442^{-}	1.095	17	1.096±0.011
(442)	1.08				
		440^{2+},442^{+}	1.055		
		442^{2+}	1.020		
		533, 422^{3+}	0.988		

Debye ring with relates to crystallographic spacies collected in table 2 for CdTe is presented in fig. 5.

IV. Discussion and conclusions

Electron diffraction patterns of both samples point out the texture nature of layers. The 6-folded axial symmetry of diffraction spots disposed on Debye rings proves very well the [111] orientation of texture, i.e. the [111] direction of grains is perpendicular to the substrate. In fact there is 12-folded symmetry. This arises from a double positioning of the crystal nucleons [10] on KCl substrate. The result of such defects is a composition of two identical diffraction patterns, one rotated of 30° in respect to the other (Fig. 4).

Results collected in Table 2 and 3 clearly separate diffractions rings arising from matrix and those which relate to diffraction caused by twinning (primary or secondary diffraction [7]). Let us consider as an example the Debye ring (311) indexed as No. 6 in Fig. 1 (CdTe), and as No. 9 ($Hg_{1-x}Cd_xTe$) in Fig. 2. Each diffraction spot on these rings has spreaded out over circular arc shape. A better inspection of the shape of such spots results in composition of three spots joining together into a triad. Two verge spots correspond to the twin 1/3 {717} = {131}, which results from any spot of the sector {131} of the matrix (middle spots in the triad). These verge twining spots are, in accordance to Eq. 1, satellites of the matrix spots {202} [11].

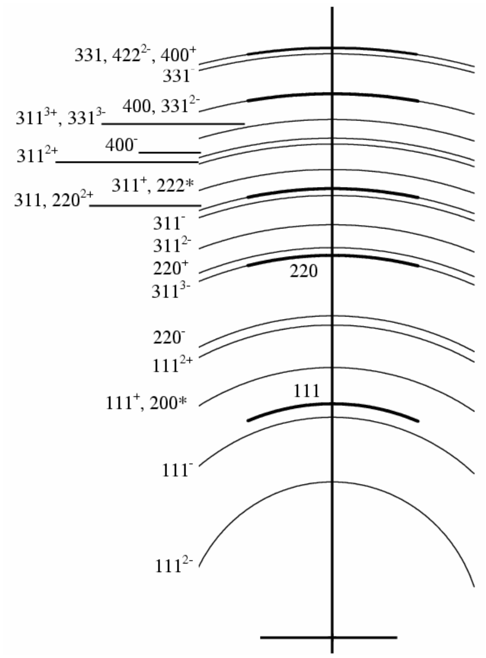

Fig. 5. Debye rings scheme for twinned CdTe, and $Hg_{1-x}Cd_xTe$ (see Table 2 and 3).

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Вивчення двійників в епітаксійних шарах CdTe і $Hg_{1-X}Cd_xTe$ методом дифракції електронів

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Структура тонких шарів CdTe та HgCdTe, отриманих методом імпульсного лазерного осадження була досліджена за допомогою електронної дифракції на проходження. Дифракційні картини мають аксіальну симетрію 12-го порядку, що свідчить про подвійну дифракцію на двійниках. Спостережувані кільця Дебая порівнювались з передбаченими у відповідності з теорією для (111) двійників у текстурованих зразках.