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THE STRUCTURE AND ORIENTATION OF CADMIUM TELLURIDE THIN FILMS DEPOSITED ONTO DIFFERENT SUBSTRATES

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The growth and the structure of evaporated thin of CdTe on an amorphous and crystalline substrates have been studied with the electron microscope and *X*-ray. The structural analysis of the electron diffraction patterns of the deposited films will be performed. The film deposited onto freshly cleaved rock-salt and carbon substrates have shown patterns of single crystalline and polycrystalline structure, respectively. The measurements were made using Philips W 1390 *X*-ray diffractometer and transmission electron microscope (Zeiss EM 10).

1. Introduction

It is well known that the structure and orientation of evaporated films are variously influenced by the formation conditions, such as residual gas pressure, deposition rate, films thickness, substrate temperature and particularly the substrate surface condition. According to published data, the CdTe films possess cubic and hexagonal phases which are metastable and lead to changes in the film characteristics with time. In the CdTe films under investigation, the hexagonal phase is absent; check of the photoelectric characteristics and film structure, six months after evaporation, showed no changes[1)].

The growth of CdTe thin films has been studied by epitaxial processes on the cleavage surface of rock-salt in vacuum using electron microscopic and electron dif-

fraction techniques. The crystallinity and structure of the films depends largely upon the intensities and species of the incident beams[2,3]. The perfection of CdTe films of different thicknesses deposited onto heated mica substrates covering the range 623—823 K was studied[4]. The most perfect monocrystalline films grow at epitaxial temperature of 573—593 K[5]. An investigation was made of the influence of condensation conditions and the state of the substrate surface on the structure of CdTe films grown in a semi-closed volume. Single crystal CdTe films grow on mica under conditions close to equilibrium when the supersaturation coefficient on the vapour $cc = 1.06$[6].

The conditions of the growth of single crystals of CdTe produce marked changes in their thermal conductivities. This study shows that the influence of some specific parameters of the growth conditions: 1 — material purity and 2—growth temperature and growth rate on the microprecipitate concentration in CdTe obtained by the travelling heater method[7]. CdTe films were sputter deposited in thicknesses of 2 to 10 μm using systematically selected deposition conditions. It is shown that the structure of these films depends on the temperature of the substrate and on the voltage during sputtering[8,9].

The intensities of the X-ray diffraction line have been measured for CdTe in the temperature range 93—393 K. The root-mean-square dynamic displacements of the lattice and of the atoms in CdTe crystals have been found to be linear functions of the temperature[10,11].

Shimaoka[12] investigated the effects of such charged particles or an electric field on the epitaxial growth, particularly the preference of epitaxial orientation of CdTe on an NaCl substrate. When the substrate was subjected to electron bombardment or a lateral electric field during the evaporation, preference of a single orientation was observed in the films. Similar effects were observed also when the electron bombardment was applied to the substrate surface immediately before or in the very early stages of the deposition or to the incident evaporation vapour. These results indicate that lattice defects of the substrate surface, produced by charged particles or an electric field, play very important roles in determining epitaxial orientation during the very early stages of film growth.

2. *Experimental procedure*

Thin films of cadmium telluride were deposited under vacuum of about 10^{-4} Pa at 300 K. CdTe can be evaporated using a tungsten boat onto glass slides, an amorphous carbon and freshly cleaved surface of rock-salt. The film thickness varied from 30 to 600 nm and the deposition rate from 7 to 12 nm/s. The film thickness was measured by Tolansky interference method[13]. The films prepared on glass slides were examined using Philips W 1390 X-ray diffractometer. The deposited CdTe on thin carbon films were ready for the examination, and the deposited films on rock-salt were then removed from the substrate after being backed with an amorphous carbon film, and observed by transmission electron microscopy and diffraction using Zeiss EM 10 electron microscope.

3. Results and discussion

It is well known that the properties of thin films are in many respects strongly different from those of the bulk material. It is generally agreed that these differences are due to a characteristic structure of the films. The analysis of the structure of CdTe films of different thicknesses and rates evaporated onto glass slides was carried out using *X*-ray diffraction technique in order to clarify the structure and the crystallite size of the deposited layers.

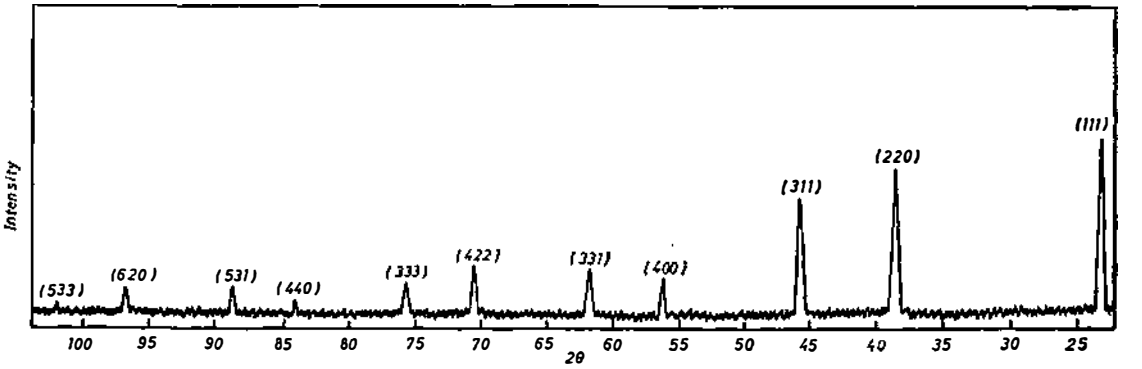


Fig. 1. *X*-ray diffractogram of CdTe powder.

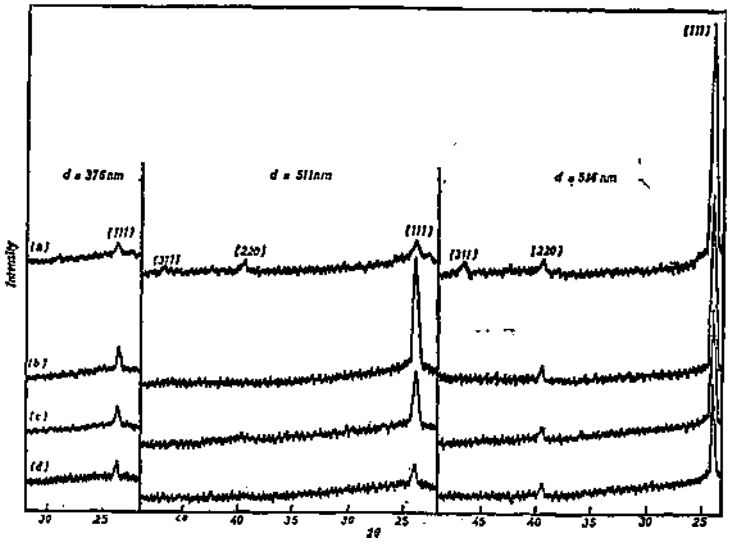


Fig. 2. *X*-ray diffractogram of a freshly deposited CdTe film of different thicknesses and rates: (a) 12 nm/s (b) 10 nm/s (c) 8.5 nm/s (d) 7 nm/s.

The corresponding X-ray powder diffraction pattern is shown in Fig. 1 and the data are listed in Table 1 compared to the ASTM card file data where good agreement appears. The X-ray diffractogram shown in Fig. 2 is for a freshly deposited CdTe film, of different thicknesses and rates. The data shows that the crystallites have an arbitrary azimuthal orientation, moreover, the degree of crystal perfection remains unchanged with a decrease in film thickness. For film thickness 376 nm the

TABLE 1.

$d_{(measured)}/10^{-8}$ cm	ASTM data		
	$d/10^{-8}$ cm	hkl	I/I_0
3.741	3.74	111	100
2.290	2.29	220	80
1.951	1.95	311	70
1.622	1.62	400	20
1.484	1.485	331	40
1.325	1.324	422	50
1.249	1.248	333	40
1.146	1.145	440	40
1.094	1.093	531	70
1.024	1.025	620	70
0.989	0.988	533	50

X-ray diffraction data of CdTe powder.

TABLE 2.

Form of B	K
For the half-breadth $B_{1/2}$	0.94
For the integral breadth B (general)	1.05
Case of a disordered layer lattice	1.84

Values for the Scherrer constant K (Ref. 23).

predominant hkl plane is (111), however, as the thickness increases and secondary nucleation occurs, additional (hkl) planes appear, namely (220) and (311) whose intensity increases with the thickness. Fig. 2 shows the X-ray diffractogram for a freshly deposited CdTe film, of different thicknesses and rates. The crystallite size S can be calculated by[14]

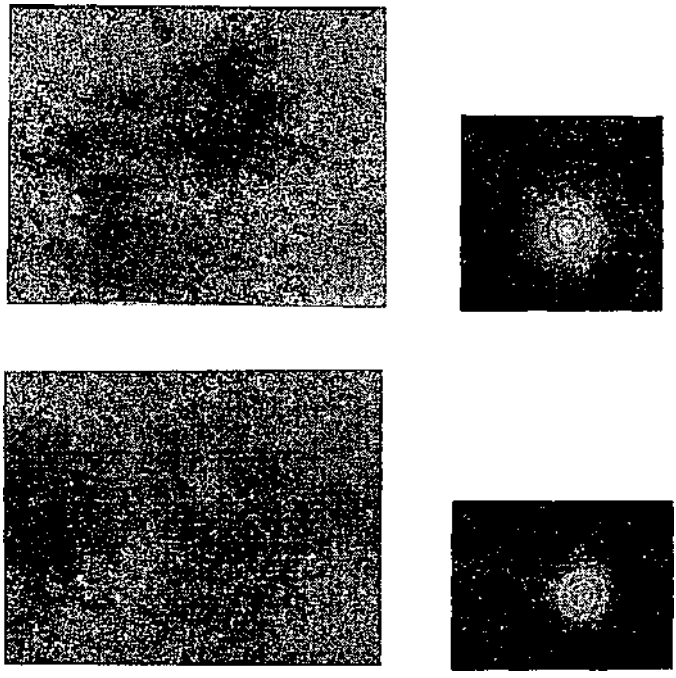
$$S = \frac{K\lambda}{B\cos\Theta} \tag{1}$$

where λ is the wavelength of the X-rays ($\lambda = 1.5404 \cdot 10^{-}10$ m) and Θ the Bragg angle ($\Theta = 0.89$). K is known as the Scherrer constant ($K = 0.94$) when B is the half-width of the diffraction $B = A/h$ with A the area subtended by the peak and h its height. The crystallite size increases as the thickness and rates increases.

On the basis of the following assumptions we can have the growth of CdTe thin films deposited on amorphous and crystalline substrates described.

1. Metal atoms impinging on a substrate are scattered, even at substrate temperatures for which the saturated-vapour pressure of the metal is far below the pressure of the vapour above the substrate[15].
2. The scattering by the substrate is not instantaneous. The atoms are absorbed and will be re-devaporated after a short time[16,17]. The average time during which an atom is adsorbed to the substrate is defined as time of adsorption[18].
3. During their stay on the substrate the atoms move over considerable distances[19].
4. As soon as condensation occurs, scattering is reduced to a negligible level[15].

It is well known that substrates of amorphous structure have been considered as neutral substrates[20]. They have practically no effect on the formation, growth and orientation of the crystal condensed on them. In the present study, no preferred orientation of CdTe crystallites deposited on amorphous carbon substrate (Fig. 3). Diffuse rings are shown in some of the given electron diffraction patterns. This character can be associated with an insufficient resolving power of the scattering crystallites and indicates small dimensions of such crystallites. The rings begin to become diffuse when the linear dimensions of the crystallites are less than 10^{-6} cm[20]. Also the non-uniform extension in the size of the crystallites in the three dimensions can lead to varying sharpness of the ringes[21].



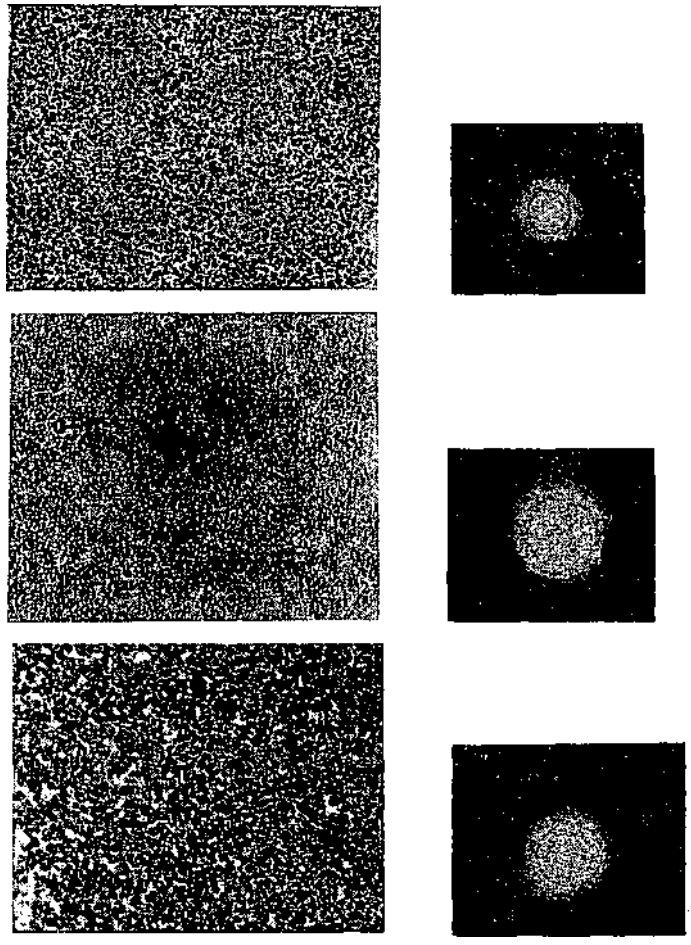


Fig. 3. Transmission electron micrographs and transmission electron diffraction patterns of CdTe deposits on carbon substrate at rate 7 nm/s.

(a) 30 nm in thickness, 26 000 X.
(b) 40 nm in thickness, 26 000 X.
(c) 50 nm in thickness, 26 000 X.
(d) 70 nm in thickness, 26 000 X.
(e) 90 nm in thickness, 40 000 X.

It is found that, at the start of growth very small and thin nuclei are formed, which, usually assumed to be spherical in shape (Fig. 3a). On increasing the thickness, the nuclei attached each other forming larger particles. Further increasing the time of evaporation aids the particles forming islands to grow and attach each other (Fig. 3 b). This attachment leads to the formation of very grains with sharp geometrical shape and larger size (Fig. 3 d). This process finally leads to the formation of CdTe crystallites in random distribution. As CdTe is of a hexagonal lattice[1], the deposited particles should possess morphological properties related to the hexagonal structure (Fig. 3 e).

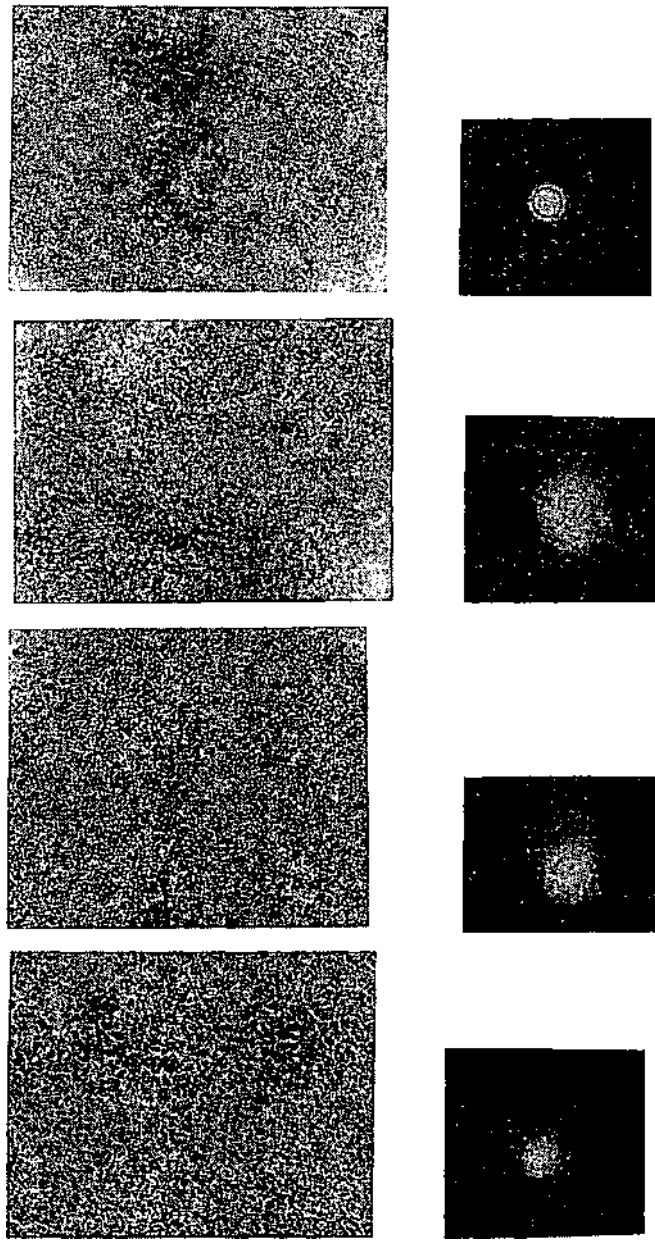


Fig. 4. Transmission electron micrographs and transmission electron diffraction patterns of CdTe deposits on a cleaved surface on a rock-salt crystal at rate 7 nm/s.

(a) 30 nm in thickness, 26 000 X.
(b) 40 nm in thickness, 26 000 X.
(c) 70 nm in thickness, 26 0000 X.
(d) 90 nm in thickness, 26 000 X.

On the other hand, it is well known generally that when the CdTe vapours are condensed on cold face of rock-salt crystals, the formed films exhibit a certain orientation with the principle directions parallel to the incident vapour beam[2,3,20]. In case of rock salt substrate, CdTe films in the initial stages of growth gave ring patterns (Fig. 4 a, b). By increasing the film thickness, the crystallinity becomes better and single crystalline pattern was obtained (Fig. 4 c). This diffraction pattern was indexed by the method of trial and error (Fig. 5). The crystal direction (uvw) which is parallel to the electron beam could be estimated[22] from

$$(uvw) = (k_1 l_2 - l_1 k_2;\ l_1 h_2 - h_1 l_2;\ h_1 k_2 - k_1 h_2). \tag{2}$$

This yielded that on crystalline substrate, oriented growth on rock-salt cleavage plane surfaces occurs such that $(111)_{CdTe} \parallel (001)_{NaCl}$.

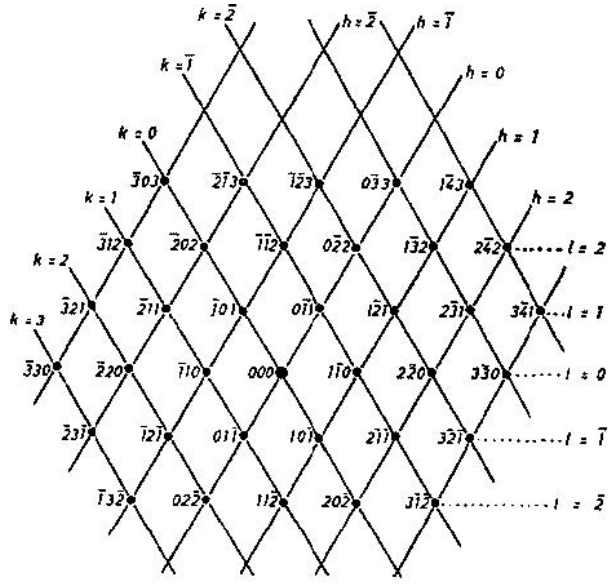


Fig. 5. Schematic diagram of the electron diffraction pattern (Fig. 4c).

A sequence of the transmission electron micrographs (Fig. 4), shows the various stages of growth of CdTe films deposited onto the freshly cleavage surface of a rock-salt. The deposition was governed by the relation between the interatomic spacing of the network of both the substrate and CdTe as well as the features of substrate surfaces. Hence, the deposition mainly occured at certain preferred sites. At the preliminary stage of growth the CdTe nuclei were small crystallites of well formed geometry (Fig. 4 a). This means that the stage of coalescence between nuclei is probably more pronounced than in the case of carbon substrate. Moreover, the rate of the crystal growth was obviously increased with increasing the thickness of the deposited films. As the time of evaporation increases, the thickness increase; this may result in the formation of aggregates of particles exhibiting a preferred orien-

tation (Fig. 4 c). Eventually the film becomes nearly continuous as shown in Fig. 4 d. This film consists of a large opaque region and small transparent one. Small holes are also observed.

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STRUKTURA I ORIJENTACIJA SLOJEVA KADMIJUM TELURIDA NAPARENIH NA RAZLIČITE PODLOGE

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Proučavani su rast i struktura naparenih tankih slojeva CdTe na amorfnim i kristaliničnim podlogama pomoću elektronskog mikroskopa te *X*-zraka. Izvršena je strukturalna analiza difrakcionih linija naparenih slojeva. Tanki sloj naparen na svježe kalanim podlogama kamene soli i ugljika pokazuje kristaliničnu, odnosno polikristaliničnu strukturu, respektivno. Mjerenja su vršena koristeći difraktometar *X*-zraka Philips W 1390 i transmisioni elektronski mikroskop (Zeiss EM 10).