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Computational Study for the Structural Change of the System $CdTe_{1-x}S_x$ Thin Film

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Abstract

Polycrystalline thin film of the graded system $CdTe_{1-x}S_x$ for $x = 0, 0.1, \ldots, 1$ are prepared by using thermal evaporation technique deposited on the glass substrate with an average thickness 3000 Å for each individual value of x. XRD technique is used with the aid of a computational program to study the phase change from cubic zinc blend structure to hexagonal wurtzite with an inversion point related to the x-value. It is found that $x = 0.1$ gives us an inversion point in the structural change from cubic to hexagonal phase.

Key Words: Thin films, ternary compound, structural behaviour and miller indices

Introduction

Recently, there has been a considerable amount of interest in the application of the graded structure such as $CdTe_{1-x}S_x$ [1],$Zn_xCd_{1-x}S$ [2], $(ZnSe)_x(CdTe)_{1-x}$ [3] and CdS_xSe_{1-x} [4] in thin film technology for various reasons. First, its possibles application in solar cell fabrication because of its high quantum efficiency. That is referred the variation in the value of energy gap as a function of x [5,6] such as in the system $CdTe_{1-x}S_x$, the value of energy gap varied within the range Eg=1.4-2.45 eV. Second, the conductivity type of CdS is only n-type, while that of CdTe is p-type with this it may be possible to produce graded heterojunction cell of n-$CdTe_{1-x}S_x$ /p-CdTe [1,7] is produced. Third, CdS and CdTe have different crystal structures; the latter being a cubic zinc blend, the former being hexagonal wurtzite [8]. The method that is used for preparing ternary or quaternary system, is thermal co-evaporation of different compounds.

Bonnet et al. [9] has succeeded in making thin films of CdS_xTe_{1-x} of various compositions $x = 0.0.1, \ldots\ldots, 1$ by co-evaporation of CdS and CdTe. In this project, we are trying to study the phase transformation from cubic to hexagonal. The correlation with

the variation of the optical energy gap, that is studied previously [10,11], was observed. It was found that at $x = 0, ..., 0.5$ the transition was the indirect one while at $x = 0.6, ..., 1$ the transition was direct with the lower value of the energy gap 1.29 eV at $x = 0.3$.

The Experimental Part

A thermal evaporation apparatus (BALZERS BAL 370) was used at high vacuum of about 1.5×10^{-5} Torr to prepare the thin film. The deposition rate was 1.8 ± 0.1 nm/sec which depends on the molecular weights of high purity compounds CdS and CdTe. The technique of two independent sources are used to evaporate the different compositions of CdTe and CdS with appropriate evaporation rates for these sources because of the different melting points of CdS 1750°C and CdTe 1041°C.

Results and discussion

X-ray diffraction patterns for the films under study, are used to specify the lattice parameters a,b and c as a function of x in the system $CdTe_{1-x}S_x$, by using a conventional horizontal diffractometer with CuKα radiation $\lambda = 1.5405$ Å. The package program POWDER is used in the specification of the crystal systems through the lattice constants and Miller indices for each phase.

Firstly, we tried to examine the crystal systems of CdTe and CdS thin films, Tables 1 & 2, by using ASTM cards. The CdTe thin film exhibited a pure cubic phase with lattice constant $a = 6.496$ Å. But the CdS film had a hexagonal phase with lattice constants $a = 3.928, c = 6.623$ Å in the presence of a little probability of cubic phase which appeared through the (200) peak as indicated by the ASTM card of CdS sample. The existence of the cubic phase together with the hexagonal one was due to the polycrystalline behaviour of thin films tending to present a multiphase structure.

Table 1. The specification of Miller indices for the CdTe sample

2θ	hkl	Crystal System
23.70	111	Cubic
33.80	112*	Hex.
39.00	220	Cubic
46.00	311	Cubic
56.65	400	Cubic
63.00	331	Cubic

As x-values varied within the range $0.1 \leq \times \leq 0.9$, the structure would change from one state to another at different phases between CdTe and CdS thin films. That demands a structural modeling for each value of x as they appeare in, Tables 3-11. It is found that there are multiphases related to the cubic and hexagonal phases, each having a different value of x in the system $CdTe_{1-x}S_x$, Table 12. The changes in the lattice constants as a function of x is shown in Fig.1. It is clear that the change in the c-values are limited, with $c = 6.5$ Å at $x = 0$ and $c = 6.62$ Å at $x = 1$, this variation satisfy a polynomial

with degree five. However Ohata et al.[8] showed that c-values varied between $c = 7.5$ Å at $x = 0$ to $c = 6.72$ Å at $x = 1$ with the semi-linear relation which satisfying Vegard's law. The inversion point at $x = 0.1$ is related to the change in a-values from cubic to hexagonal phase which exhibited an abrupt change in the a-value from $a = 6.5$ Å at $x = 0$ to $a = 4.8$ Å at $x = 0.1$. This was not in agreement with the inversion point from the indirect energy gap to the direct one that was obtained at $x = 0.5$ as reported previously [10,11].

Table 2. The specification of Miller indices for CdS sample

2θ	hkl	Crystal System
24.80	100	Hexagonal
26.50	101	Hexagonal
27.90	002	Hexagonal
31.05	200	Cubic
36.65	102	Hexagonal
43.50	110	Hexagonal
47.80	103	Hexagonal

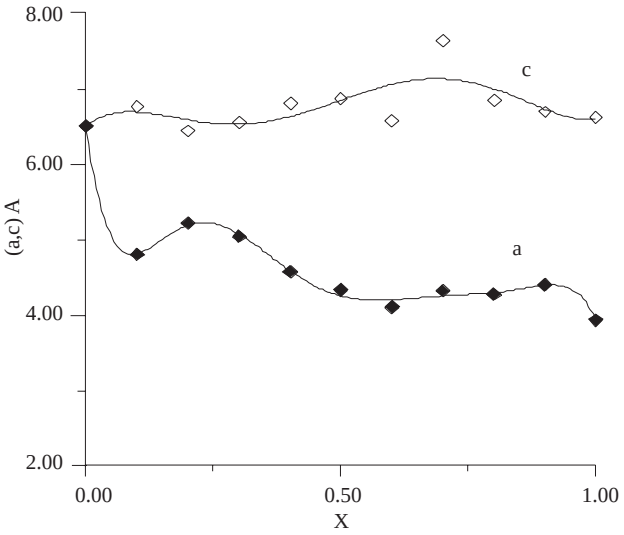

Figure 1. The changes in the lattice constants as a function of (x) in $CdTe_{1-x}S_x$

Table 3. The specification of Miller indices for $CdTe_{0.9}S_{0.1}$ sample

2θ	hkl	Crystal System
23.90	111	Cubic
24.85	100	Hexagonal
26.80	003*	Hexagonal
27.15	101	Hexagonal
39.20	220	Cubic
46.45	311	Cubic
47.70	103	Hexagonal

Table 4. The specification of Miller indices for $CdTe_{0.8}S_{0.2}$ sample

2θ	hkl	Crystal System
24.00	111	Cubic
26.70	101	Hexagonal
27.75	002	Hexagonal
39.30	220	Cubic
43.80	110	Hexagonal
46.45	311	Cubic

Table 5. The specification of Miller indices for $CdTe_{0.7}S_{0.3}$ sample

2θ	hkl	Crystal System
24.15	111	Cubic
26.40	002	Hexagonal
27.65	200	Cubic
30.75	102	Hexagonal
40.00	220	Cubic
42.40	200	Hexagonal
44.10	201	Hexagonal
45.65	103,112	Hexagonal

Table 6. The specification of Miller indices for $CdTe_{0.6}S_{0.4}$ sample

2θ	hkl	Crystal System
24.25	111	Cubic
24.80	101	Hexagonal
30.50	102	Hexagonal
31.85	110	Hexagonal
40.30	003*	Hexagonal
44.00	200	Hexagonal
44.70	201	Hexagonal
45.00	103	Hexagonal
47.00	112	Hexagonal

Table 7. The specification of Miller indices for $CdTe_{0.5}S_{0.5}$ sample

2θ	hkl	Crystal System
24.00	111	Cubic
24.80	101	Hexagonal
26.00	002	Hexagonal
32.55	102	Hexagonal
32.85	102	Hexagonal
35.10	110	Hexagonal
40.35	111*	Hexagonal
44.15	200	Hexagonal
45.00	103	Hexagonal
48.00	112,201	Hexagonal

Table 8. The specification of Miller indices for $CdTe_{0.4}S_{0.6}$ sample

2θ	hkl	Crystal System
24.90	100	Hexagonal
26.05	101	Hexagonal
28.65	002	Hexagonal
36.20	102	Hexagonal
37.40	110	Hexagonal
42.00	003*	Hexagonal
44.30	200	Hexagonal
45.50	201	Hexagonal
48.40	112,103	Hexagonal

Table 9. The specification of Miller indices for CdTe0.3S0.7 sample

2θ	hkl	Crystal System
24.85	111	Cubic
25.95	100	Hexagonal
26.40	101	Hexagonal
26.50	101	Hexagonal
27.10	002	Hexagonal
31.00	102	Hexagonal
33.10	110	Hexagonal
46.00	003*	Hexagonal

The variation in a-values, in the range of $x = 0.2 - 0.6$, appeared as a transitional state from cubic to hexagonal. This behaviour, confirmed through the XRD pattern of hexagonal phase, has stronger peaks than the cubic phase. These results confirm the enhancement of a hexagonal phase at $x \geq 0.1$ as shown in, Table 12. It is clear that when x is increased over 0.1, the ratio of hexagonality is also increased, emphasizing the multiphase presence of $CdTe_{1-x}S_x$ for $0.1 \leq \times \leq 0.9$. This is in contradiction with Ohata

et al. [8] which shows that the presence of single phase is due to a phase transformation from CdTe to CdS. When the range of x has a value 0.6-1, it seems to exhibit a semi-linear behaviour towards the end point at $x = 1$ with a pure hexagonal phase and the presence of a foreign peak labelled by (200) and is related to the cubic phase as indicated in Table 2. The overall behaviour of curve (a) is represented by a polynomial of degree seven, but in a previous study the behaviour was satisfied the Vegard's law [8].

Table 10. The specification of Miller indices for $CdTe_{0.2}S_{0.8}$ sample

2θ	hkl	Crystal System
24.00	111	Cubic
24.70	100	Hexagonal
25.35	002	Hexagonal
26.15	101	Hexagonal
27.20	102	Hexagonal
28.90	003*	Hexagonal
29.25	003*	Hexagonal
35.10	110	Hexagonal
42.90	103	Hexagonal

Table 11. The specification of Miller indices for $CdTe_{0.1}S_{0.9}$ sample

2θ	hkl	Crystal system
24.60	111	Cubic
24.80	100	Hexagonal
25.70	101	Hexagonal
26.30	002	Hexagonal
28.00	200	Cubic
31.60	102	Hexagonal
36.20	110,003*	Hexagonal
43.45	111*	Hexagonal
47.90	201,200	Hexagonal

The peaks marked by star in the following tables were found not to depend on both pure CdTe and CdS as appeared in ASTM-cards. These peaks may be related to a new phase mixed with cubic and hexagonal phases, and it may also be an intermediate state between them. The most significant of those peaks is labelled by (003) which appeared first with $2\theta = 26.8$ at $x = 0.1$. Obviously, the (003) plane was shifted toward high value of 2θ up to $2\theta = 46$ as x increased within the range $0.1 \leq \times \leq 0.7$. That was emphasized with the intermidate state within the range $x = 0.2 - 0.6$ as shown in Fig.1. As x exceeded 0.7, the plane was shifted towards a lower value of 2θ such as $2\theta = 28 - 36.2$ for $x = 0.8, 0.9$, respectively. That was emphasized with the enhancement of hexagonal phase in the compositions near CdS composition.

Table 12. The effects of the concentration (x) in the composition of $CdTe_{1-x}S_x$ on the structural phase.

x	Cubic ratio	Hexagonal ratio	a (°A)	c (°A)
0.0	100%		6.50	
0.1	40%	60%	4.80	6.76
0.2	50%	50%	5.22	6.44
0.3	37%	63%	5.04	6.56
0.4	10%	90%	4.57	6.81
0.5	10%	90%	4.33	6.86
0.6		100%	4.10	6.58
0.7	10%	90%	4.32	7.63
0.8	10%	90%	4.27	6.85
0.9	20%	80%	4.40	6.69
1.0	15%	85%	3.93	6.62

Conclusion

These results depend on the simulation of indexing because each system contains ternary compounds which are considered a good tool for determining structural change. It is very important to specify and correlate it with the presence of the multilayers of graded structure of $CdTe_{1-x}S_x$. The specification is more significant in the representation of graded structure through the preparation of a heterojunction solar cell by a tendum structure. Therefore, it is considered a good tool to investigate the presence of the graded $CdTe_{1-x}S_x$ system as a function of x through the appearance of most peaks which were observed on the XRD patterns.

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