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Structural analysis of cadmium sulfide thin film prepared by vacuum evaporation by using the FullProf program

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ABSTRACT

Using the Fullprof program we analyzed X-ray diffraction of CdS thin film prepared by vacuum evaporation on glass substrate. The program fitted and refined the experimental XRD data by two methods; Le Bail fitting and Rietveld refinement. Experimental profiles of the XRD data were fitted by modified Thompson-Cox-Hastings pseudo-Voigt functions. The analyses revealed that CdS thin film has cubic (zinc blend) phase structure. A good agreement between experimental and simulated patterns was obtained. The values of lattice constant (*a*), space group, atomic coordinates (*x*, *y*, *z*), isotropic temperature factors (B_{iso}), occupation (*Occ.*), multiplicity (*m*), bond length and bond angle between Cd and S atoms were calculated for CdS thin film. The FullProf program drew the structure in accordance with atomic positions for CdS thin film as three-dimensional projection which demonstrated that Cd and S atoms are formed in a tetrahedral configuration. The obtained data from the FullProf refinement were used to calculate the average crystallite size and related parameters for CdS thin film.

KEYWORDS

CdS thin film;
Structural analysis;
Fullprof program;
Le bail;
Rietveld;
Refinement.

INTRODUCTION

Cadmium sulfide (CdS), with its large band gap (2.42 eV), is being widely studied because of its use as a window layer in many types of solar cells in conjunction with absorbers such as CdTe[1] and $CuInSe_2$[2]. CdS thin films have been prepared by diverse techniques such as vacuum evaporation[3], spray pyrolysis[4], electrodeposition[5], chemical bath deposition (CBD)[6] and dc-sputtering[7].

A lot of papers have been published on CdS thin films in terms of many properties, specially, optical and structural properties. In terms of structure, it has been reported that CdS can exist in cubic (zinc blende) phase[8-13], hexagonal phase[14-16] or mixed of the two phases[17, 18], depending on the synthesis conditions.

Standard data from JCPDS shows that CdS XRD pattern show peak at 2θ = 26.14° which is associated with the mixture of hexagonal (0 0 2) and cubic (1 1 1) planes, the peak at 2θ =36.2° corresponds to the hexagonal (1 0 2) plane, the peak at 2θ=43.8° is associated with the hexagonal (1 1 0) and cubic (2 2 0) planes and the peak at 2θ=66.42° corresponds to the hexagonal (2 0 3). The peaks (0 0 2) and (1 1 0) of the hexagonal structure are similar to the (1 1 1) and (2 2 0) peaks of cubic one[17]. From these data it is not possible to determine whether the film is present in the hexagonal phase, cubic phase, or a mixture of the two phases[18]. Nevertheless it is possible to conclude that the films are highly textured in either[0 0 2] or[1 1 1] direction.

As our knowledge, the achieved studies on CdS thin films used conventional methods to determine the structure of CdS thin film. These studies were not able to confirm the exact structure of CdS (cubic, hexagonal or mixed of the two phases) by the XRD spectra. Also, there is no enough studies on the structure details (whether cubic or hexagonal) like atomic positions, isotropic temperature factors, occupation, multiplicity, bond lengths and bond angles. Therefore, in this paper we employed Le Bail fitting and Rietveld refinement with the FullProf modern program to elucidate crystal structure of CdS thin film prepared by vacuum evaporation method, to give some important details about this structure and to calculate the crystallite size of CdS thin film accurately.

THEORY

The refinement program; FullProf[19] can be used to treat the obtained data from XRD measurements by employing two methods; Rietveld[20] and Le Bail[21]. Rietveld refinement uses a least-squares minimization technique that, as any local search technique, is easily stuck in false minima. Besides, correlation between model parameters, or a bad starting point, may easily cause divergence in early stages of the refinement. The user must be aware of the way he can control the refinement procedure: the number of parameters to be refined, fixing parameters, making constraints, etc. The Le Bail method is a popular method for whole-pattern decomposition (profile matching) methods, which can be adjusted without prior knowledge of the structure (needs only good starting cell and profile parameters). In this method, the reflection intensity values are initially set to arbitrary values. The intensities evolve iteratively, where reflection intensity values are arbitrarily assigned to estimates obtained by apportioning data values amongst the contributing reflections. Other parameters including background function, unit cell, and peak profile parameters can be refined simultaneously with the Le Bail intensity extraction. The Le Bail and other whole-pattern decomposition (profile matching) methods are often the only way to apply full pattern methods when structures are not known or are difficult to describe, such as with disordered structures. These methods may also be used preferentially to the Rietveld method when experimental artifacts are difficult to model, as may be the case when in situ diffraction cells are used. In some cases, in particular when the structural model is very crude, it is advisable to analyze first the pattern with the Le Bail method in order to determine accurately the profile shape function, background and cell parameters before running the Rietveld method. Le Bail fitting is preferable to initially performed because of the capability of the method for the fast observation of lattice dynamics. The instrument zero, the lattice parameters, asymmetry parameters and the peak shape parameters can be refined in the first by Le Bail method. Subsequently, Rietveld fitting can be performed and the same parameters will refined again beside other parameters like atomic coordination, temperature factors, occupation, multiplicity, bond lengths, and angles.

Temperature factors or thermal parameters describe not only the time-averaged temperature dependent movement of the atoms about their mean equilibrium positions (dynamic disorder), but also their random distribution over different sets of equilibrium positions from one unit cell to another, representing a deviation from perfect periodicity in the crystal (static disorder) which is not great enough to be resolved into distinct alternative sites), and so they should rather be called “atomic displacement parameters”[22]. Multiplicity (*m*) of atom site is number of atoms in position. It is related to the site occupancy factor or occupation (*Occ.*) which is used in some cases such as disordered structures because a site may be occupied by an atom in some unit cells and not in others[22]. Occupation for fully occupied lattice sites is equal to m/M where m is the multiplicity of the position, special or general, and M is the multiplicity of the general position in the particular space group. The value of *m* ranges in general from 1 to *M*[20].

The experimental profiles can be fitted by modified Thompson-Cox-Hastings pseudo-Voigt functions[23]:

$$H_G = (U\tan^2\theta + V\tan\theta + W + Z/\cos^2\theta)^{1/2} \qquad (1)$$

and

$$H_L = X\tan\theta + Y/\cos\theta \qquad (2)$$

where H_G is the Gaussian component of the peak width, H_L is the Lorentzian component of the peak width, *U* is the Gussian isotropic microstrain parameter, θ is the Bragg angle, *Z* is the Gussian isotropic crystallite size parameter, *X* is the Lorentzian isotropic microstrain parameter, and *Y* is the Lorentzian isotropic crystallite size parameter.

The average crystallite size (*D*) can be calculated from the full width at half maximum (FWHM) of the peaks using the Debye–Scherrer equation[24]:

$$D = \frac{0.9\lambda}{\beta\cos\theta} \qquad (3)$$

where λ is the X-ray wavelength, β is the full width at half maximum (FWHM) of the peak (in radians) and θ is the Bragg angle for the corresponding plane. The dislocation density (δ), which defined as the length of dislocation lines per unit volume, can be estimated by using the following equation[25]:

$$\delta = \frac{1}{D^2} \qquad (4)$$

The thickness (*t*) of the thin film can be calculated with the help of a weight difference method employing a sensitive electronic microbalance; in this method the substrate will be weighted before (m_1) and after the deposition (m_2) and the thickness of the film can be obtained using the formula:

$$t = \frac{m_2 - m_1}{\rho A} \qquad (5)$$

where ρ is the density of the film material and *A* is the area of the film (in cm^2). The number of crystallites per unit area (*N*) of the film can be determined using the following equation[26]:

$$N = \frac{t}{D^3} \qquad (6)$$

Also, the strain (ε) of the film can be determined with the use of the following equation[26]:

$$\varepsilon = \frac{\beta\cos(\theta)}{4} \qquad (7)$$

EXPERIMENTAL PROCEDURES

Sample preparation

Cadmium sulfide (CdS) thin film was prepared by evaporating 99.999% pure crystal onto well-cleaned glass substrate from a molybdenum boat. The evaporation was made using a conventional vacuum coating unit (Edwards E306) at a vacuum of 10^{-5} Torr. The film was grown at 20 RºC substrate temperature.

X-ray diffraction measurement

The X-ray diffraction (XRD) measurement was achieved at room temperature (20 RºC) by using Diano PW 1370, CoKα radiation, λ= 0.1793 nm and were swapped from 2θ= 5º to 2θ= 90º with step of 0.1º

Treatment of the XRD data

The obtained data from XRD measurement for CdS thin film were treated by the FullProf program using the modified Thompson-Cox-Hastings pseudo-Voigt functions (equations 1 and 2) by two methods (Le Bail then Rietveld). Firstly, Le Bail method was used to refine the global parameters (profile asymmetry, background, and specimen displacement) in the first step. Then, Lattice parameters, preferred orientation, asymmetry parameters, and the peak shape parameters were refined in the second step. In the last cycle, when the discrepancy factor R_{wp} reached a minimum value, all the parameters were refined simultaneously looking for a minimum goodness of fit index χ^2. After that, Rietveld method was used to refine the global parameters (profile asymmetry, background, and specimen displacement) again in the first step of this refinement. In the next step, the structural parameters (atomic coordination, parameters of specimen profile breadth, lattice parameters, temperature factors, preferred orientation, site occupancy factors, bond lengths, and angles) were refined in sequence modes. In the last cycle, when the discrepancy factor R_{wp} reached a minimum value, all the parameters (global and structural) were refined simultaneously looking for a minimum goodness of fit index χ^2.

RESULTS AND DISCUSSION

Figure 1 shows the X-ray diffraction pattern of the obtained CdS thin film. The figure shows that the film is polycrystalline in nature. Also, the figure shows a predominant peak at $2\theta = 30.95^o$ and small peak at $2\theta = 64.50^o$ which could be indicated as scattering from the (1 1 1) and (2 2 2) cubic plans or (0 0 2) and (0 0 4) hexagonal plans respectively. The refinement by the FullProf program confirmed that the exact structure of the obtained CdS thin film is cubic (zinc blend phase), and is not hexagonal. This for two reasons: first the other peaks of hexagonal phase are not apparent; and second the FullProf program was not able to refine the structure with hexagonal phase conditions whether by Le Bail method or by Rietveld method.

Because all parameters that refined by the two methods (Le Bail and Rietveld) do not differ considerably and Rietveld method refined more parameters, only final results of Rietveld method will be displayed. Figure 2 shows the outcome of the

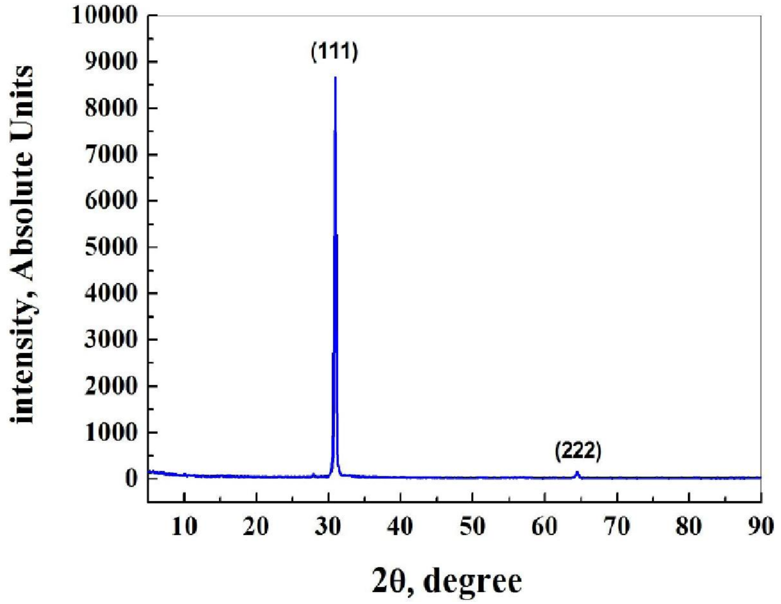

Figure 1 : XRD pattern of CdS thin film prepared by vacuum evaporation on glass substrate.

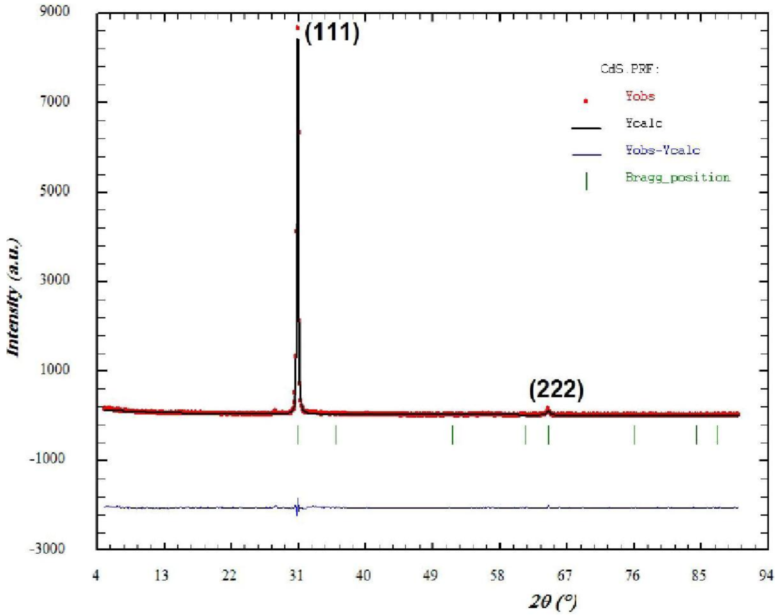

Figure 2 : The outcome of the FullProf program for CdS thin film.

TABLE 1 : Crystal data calculated by the FullProf program for CdS thin film

Chemical formula	CdS
Formula weight (M_r), g mol^{-1}	144.477
Range of the distance between planes *d(hkl)*, Å	3.360163-1.301386
Crystal system	Cubic
Space group	*F-43m*
Number of space group	216
Point group	*-43m*
Bravais lattice	*fcc*
Unit cell dimension (*a*), Å	5.82006 ± 0.00173
Unit cell volume (*V*), Å^3	197.143 ± 0.102
Number of molecules in the unit cell (z)	4

TABLE 2 : Atomic parameters (fractional coordinates, isotropic temperature factor, occupation, and multiplicity) calculated by the FullProf program for CdS thin film

Atom	Fractional coordinates			Isotropic temperature factor ($B_{iso.}$), Å^2	Occupation (*Occ.*)	Multiplicity (*m*)
	x	*y*	*z*			
Cd(1)	0.0000	0.0000	0.0000	0.0324	1.0000	4
Cd(2)	0.0000	0.5000	0.5000	0.0100	1.0000	4
Cd(3)	0.5000	0.0000	0.5000	0.0240	1.0000	4
Cd(4)	0.5000	0.5000	0.0000	0.0095	1.0000	4
S(1)	0.7500	0.7500	0.2500	0.0042	1.0000	4
S(2)	0.2500	0.2500	0.2500	0.0219	1.0000	4
S(3)	0.2500	0.7500	0.7500	0.0086	1.0000	4
S(4)	0.7500	0.2500	0.7500	0.0085	1.0000	4

FullProf program in which the observed peaks, the calculated ones, and their difference in profile of CdS thin film are presented. The observed data are given as points and calculated data are shown as solid line. Difference between observed and calculated data is shown as bottom line. The vertical lines represent the Bragg's allowed peaks. The XRD peaks were generated by using *F-43m* space group, i.e. in face centered cubic (fcc) symmetry. The crystal data obtained from the FullProf program calculations are listed in TABLE 1.

The results in TABLE 1 have very good agreements with literatures[8-13] and with the JCPDS data (Card No. 5-0566). Also, the values of discrepancy factors obtained from the FullProf program calculations are $R_p = 10.8$, $R_{wp} = 17.3$, $R_{exp} = 12.42$ and the goodness of fit index $\chi^2 = 1.94$. These values reveal the good quality of refinement in this work. Moreover, the correctness of the refinement is indicated by checking the atomic parameters, bond lengths and angles as we will present them at once.

The refined values of atomic fractional coordinates, isotropic temperature factor, occupation, and multiplicity are presented in TABLE 2. The atoms positions gave the possibility to determine bond lengths for Cd*i*-S*i* where *i* = 1, 2, 3, 4 (four molecules in the unit cell). These calculated bond lengths of CdS thin film are presented in TABLE 3. In addition, the calculated bond angles for S*i*-Cd*i*-S*i* and Cd*i*-S*i*-Cd*i* where *i* = 1, 2, 3, 4 in CdS thin film are presented in TABLE 4. From TABLES 2, 3 and 4, one can see that the unit cell has four CdS molecules and every sulfur (S) atom is surrounded by four cadmium (Cd) atoms (or vice-versa). All Cd-S distances, S-Cd-S and Cd-S-Cd angles are equals. This means that the nearest neighbor connections of cadmium and sulfur atoms have the same bond lengths and angles. The values of Cd-S distance (2.52016 Å), S-Cd-S and Cd-S-Cd angle (109.471 °) have very good agreements with literature[27].

By using the obtained values of unit cells, atomic positions, bond lengths and bond angles, the FullProf

TABLE 3 : Bond lengths calculated by the full prof program for CdS thin film

Bond	Length, Å	Bond	Length, Å
Cd(1)-S(1)	2.52016(5)	Cd(3)-S(1)	2.52016(5)
Cd(1)-S(2)	2.52016(5)	Cd(3)-S(2)	2.52016(5)
Cd(1)-S(3)	2.52016(5)	Cd(3)-S(3)	2.52016(5)
Cd(1)-S(4)	2.52016(5)	Cd(3)-S(4)	2.52016(5)
Cd(2)-S(1)	2.52016(5)	Cd(4)-S(1)	2.52016(5)
Cd(2)-S(2)	2.52016(5)	Cd(4)-S(2)	2.52016(5)
Cd(2)-S(3)	2.52016(5)	Cd(4)-S(3)	2.52016(5)
Cd(2)-S(4)	2.52016(5)	Cd(4)-S(4)	2.52016(5)

TABLE 4 : Bond angles calculated by the full prof program for CdS thin film

Bond	Angle, °	Bond	Angle, °
S(1)-Cd(1)-S(2)	109.471(4)	Cd(1)-S(1)- Cd(2)	109.471(4)
S(1)-Cd(1)-S(3)	109.471(4)	Cd(1)-S(1)- Cd(3)	109.471(4)
S(1)-Cd(1)-S(4)	109.471(4)	Cd(1)-S(1)- Cd(4)	109.471(4)
S(2)-Cd(1)-S(3)	109.471(4)	Cd(2)-S(1)- Cd(3)	109.471(4)
S(2)-Cd(1)-S(4)	109.471(4)	Cd(2)-S(1)- Cd(4)	109.471(4)
S(3)-Cd(1)-S(4)	109.471(4)	Cd(3)-S(1)-Cd(4)	109.471(4)
S(1)-Cd(2)-S(2)	109.471(4)	Cd(1)-S(2)-Cd(2)	109.471(4)
S(1)-Cd(2)-S(3)	109.471(4)	Cd(1)-S(2)-Cd(3)	109.471(4)
S(1)-Cd(2)-S(4)	109.471(4)	Cd(1)-S(2)-Cd(4)	109.471(4)
S(2)-Cd(2)-S(3)	109.471(4)	Cd(2)-S(2)-Cd(3)	109.471(4)
S(2)-Cd(2)-S(4)	109.471(4)	Cd(2)-S(2)-Cd(4)	109.471(4)
S(3)-Cd(2)-S(4)	109.471(4)	Cd(3)-S(2)-Cd(4)	109.471(4)
S(1)-Cd(3)-S(2)	109.471(4)	Cd(1)-S(3)-Cd(2)	109.471(4)
S(1)-Cd(3)-S(3)	109.471(4)	Cd(1)-S(3)-Cd(3)	109.471(4)
S(1)-Cd(3)-S(4)	109.471(4)	Cd(1)-S(3)-Cd(4)	109.471(4)
S(2)-Cd(3)-S(3)	109.471(4)	Cd(2)-S(3)-Cd(3)	109.471(4)
S(2)-Cd(3)-S(4)	109.471(4)	Cd(2)-S(3)- Cd(4)	109.471(4)
S(3)-Cd(3)-S(4)	109.471(4)	Cd(3)-S(3)-Cd(4)	109.471(4)
S(1)-Cd(4)-S(2)	109.471(4)	Cd(1)-S(4)-Cd(2)	109.471(4)
S(1)-Cd(4)-S(3)	109.471(4)	Cd(1)-S(4)-Cd(3)	109.471(4)
S(1)-Cd(4)-S(4)	109.471(4)	Cd(1)-S(4)-Cd(4)	109.471(4)
S(2)-Cd(4)-S(3)	109.471(4)	Cd(2)-S(4)-Cd(3)	109.471(4)
S(2)-Cd(4)-S(4)	109.471(4)	Cd(2)-S(4)-Cd(4)	109.471(4)
S(3)-Cd(4)-S(4)	109.471(4)	Cd(3)-S(4)-Cd(4)	109.471(4)

program drew the structure visualization (the structure in accordance with atomic positions) for CdS thin film as three-dimensional projection which is clear in Figure 3. This figure shows that only half of the tetrahedral sites (i.e. four of the eight octants of the cube) are occupied by S. The tetrahedral shape of CdS (one S atom surrounded by four Cd atoms) in accordance with atomic positions is clear in Figure 4.

From TABLES 1 to 4 and Figures 1 to 4, one can see that the obtained CdS thin film in this work has cubic (zinc blend) structure. This structure is based on a face centered cubic (fcc) lattice of cations (Cd) with an interpenetrating fcc lattice of anions (S) or vice-versa. Cd atoms occupy one of the two types of tetrahedral holes present and S atoms occupy the other. The nearest neighbor connections are similar (have the same bond lengths and angles).

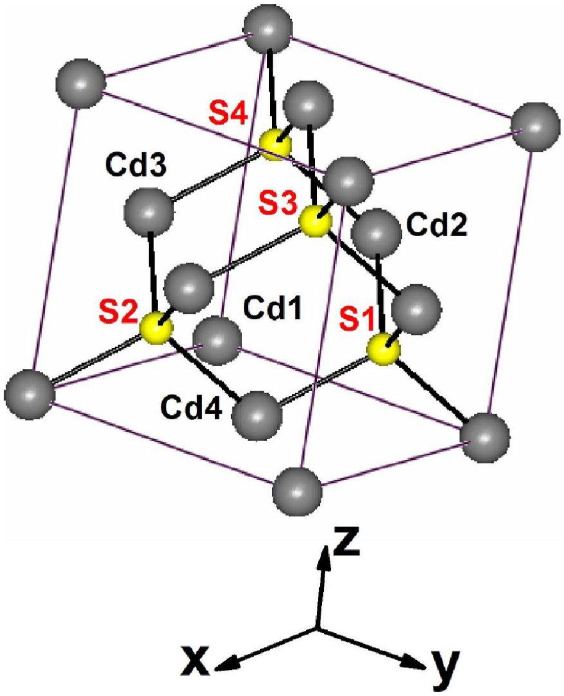

Figure 3 : The structure of CdS thin film in accordance with atomic positions

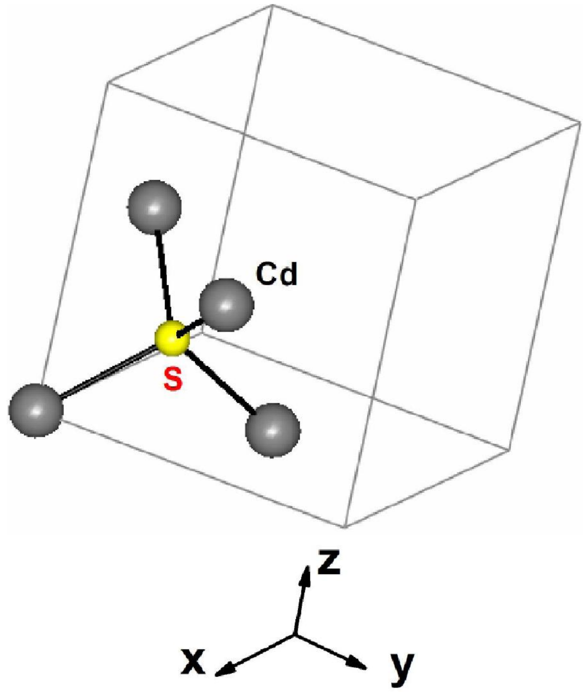

Figure 4 : The tetrahedral structure of closest neighbors in the CdS lattice

The structure has four asymmetric units in its unit. Each ion is four coordinate and has local tetrahedral geometry. In zinc blende structure, the cell looks the same whether one start with anions or cations on the corners, i.e. one can switch the anion and cation positions in the cell and it doesn't matter as in NaCl and in ZnS beside CdS. In fact, replacement of both Cd and S with carbon (C) gives the known diamond structure. The diamond structure refers to the particular lattice in which all atoms are of the same species, such as carbon, silicon or germanium. The zinc blende structure differs from the diamond structure only in that there are two different types of atoms in the lattice of the zinc blende structure while there is only one type of atoms in the lattice of the diamond structure. The important feature of both the diamond and the zinc blende structures is that the atoms are joined together to form a tetrahedron[28].

For the plane (1 1 1), the values of 2θ and β (FWHM) were extracted from the FullProf refinement data. Then, by using equation (3) and substituting λ with its value (0.1793 nm), the average crystallite size (D) of CdS thin film was calculated. The dislocation density (δ) was calculated for CdS thin film by using equation (4). The thickness (t) of CdS thin film was calculated by using equation (5) where the density (ρ) of CdS material = 4.84 g/cm^3[11]. The number of crystallites per unit area (N) of CdS thin film was determined with the use of equation (6). Finally, the strain (ε) of CdS thin film was determined with the use of equation (7). The average crystallite size and related parameters obtained from the peak at 30.948º, (1 1 1) cubic plane, for CdS thin film are summarized in TABLE 5.

One can see from TABLE 5 that the average crystallite size (D) of CdS thin film (35.40 nm) is less than 100 nm, and therefore the obtained thin film in this work has crystallites with size in nano range. Since the dislocation density (δ) is a measure of the amount of defect in the crystal, its small value obtained in this work, as in TABLE 5, confirmed the good crystallinity of the obtained CdS thin film. Because Jassim et al.[16] used conventional methods to obtain β (FWHM) value in order to calculate the average crystallite size and related parameters for the same peak at 30.948º, our obtained values in TABLE 5 have more accuracy. Also the same paper[16] said that the structure of CdS thin film is hexagonal according to the used conventional methods, but in the present work the modern FullProf program confirmed that the structure is cubic (zinc blende) in spite of the similarity of the sample prepa-

TABLE 5 : Structural parameters of CdS thin film obtained from (1 1 1) peak

2θ, °	β, rad	Crystallite size (D), nm	Dislocation density ($\delta\times10^{15}$), lines/m^2	Thickness (t), nm	Number of crystallites per unit area ($N\times10^{15}$), m^{-2}	Strain ($\varepsilon\times10^{-4}$)
30.948	0.00473	35.40	0.798	1600	36.07	11.40

ration methods and XRD data.

CONCLUSIONS

The refinement of the XRD data by the FullProf program confirmed that CdS thin film, prepared by vacuum evaporation on glass substrate, has the cubic (zinc blende) crystal structure. The structure has *F-43m* space group, 5.82006 Å lattice constant and four CdS molecules in the unit cell. The drawn structure by the FullProf program, in accordance with atomic positions, for CdS thin film can show clearly that cadmium (Cd) and sulfur (S) atoms are formed in a tetrahedral configuration. Every S atom is surrounded by four Cd atoms and vice-versa. All Cd-S distances, S-Cd-S and Cd-S-Cd angles are equals (2.52016 Å and 109.471°). Each atom is four coordinate and has local tetrahedral geometry. The cell looks the same whether one start with Cd or S on the corners. Replacement of both Cd and S with carbon (C) gives the known diamond structure. The average crystallite size of CdS thin film obtained from the plane (1 1 1) is 35.40 nm. It is less than 100 nm, and therefore the obtained CdS thin film has crystallites in nano range.

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