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Thickness dependence of structural and optical properties of cadmium iodide thin films

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ABSTRACT

Structural and optical properties as a function of film thickness have been studied for the thermally evaporated cadmium iodide (CdI_2) films. According to XRD structure, the thickness of investigated films extends from 272 to 696 nm, showing hexagonal structure and good *c*-axis alignment normal to glass substrate plane. Both of crystallite size and lattice strain have been determined in terms of Voight method of the main peak. The optical constants, refractive index (n), and extinction coefficient (k) have been determined using envelope method. The optical absorption data indicates an allowed direct inter – band transition near the absorption edge with an optical energy gap that decreases continuously from 3.572 to 3.767 eV. Both of optical constants and energy gap show thickness dependence that can be explained in terms of structure parameters, crystallite size, and lattice strain.

1. Introduction

Cadmium iodide, CdI_2, is a chemical compound of cadmium and iodine. It is notable for its crystal structure, which is typical for compounds of the form MX_2 with strong polarization effects [1]. The basic structure consists of an infinite hexagonal sheet of Cd atoms sandwiched between two similar sheets of I atoms, the Cd atoms being octahedrally coordinated. These three sheet sandwiches are then stacked to form the three-dimensional compound. CdI_2 is a well-known material having a number of polytypes as high as 200 out of which only very few are commonly occurring [2]. CdI_2 is used in lithography, photography, electroplating and the manufacturing of phosphors. The reported studies on CdI_2 concerning structure and optical properties are quite diverging. Studies on CdI_2 films regarding structure [3,4] and optical properties [5,6] are quite limited. The optical properties were shown to have a strong correlation with the microstructure parameters. The growth of crystallize size and its distribution, as stated, depends on film thickness and deposition rate. Many publications have been determined both refractive index and thickness of thin films by measuring reflectance and transmittance using spectrophotometer [7–11] and measuring psi and delta using spectroscopic ellipsometry [12–14]. Both of which were a powerful techniques to investigate the optical response of materials. Therefore, we thought it worthwhile to carry out detailed optical studies of transmittance and reflectance spectra in both transparent and strong absorption regions for determination the optical constants (refractive index and absorption coefficient thus energy gap) of CdI_2 thin films with high precision. The present work deals with: (1) calculation of structural parameters of both of crystallite size and lattice strain of different thickness of CdI_2 in terms of Voight method, (2) calculation of thickness and refractive index using envelope method suggested by Swanepoel, (3) calculation of direct optical band gap using transmission and reflection spectra in the strong absorption region, and (4) interpretation of change in optical constants in terms of structural parameters.

2. Experimental details

CdI_2 was purchased from Sigma Aldrich Company and used as received without any further purification. CdI_2 thin films of different thickness were evaporated by thermal evaporation system (model E-306A, England) on clean glass substrates.

The base vacuum pressure was about 2×10^{-5} Torr. The evaporation rate as well as the film thickness was controlled using a quartz crystal monitor (FTM4, Edwards). The deposition rate was constantly maintained at 10 Å/s throughout the sample preparation. Such a low deposition rate produces a film composition, which is very close to that of the bulk starting material. The distance between filament source and substrate holder was 21 cm to avoid any heating effect during the evaporation of CdI_2.

The structure and phase purity of the powder and as-deposited films were measured at room temperature by means of X-ray powder diffraction (XRD) Philips X-ray diffractometer (model-X' pert) with Cu $K\alpha_1$ radiation ($\lambda = 1.54056$ Å). The data

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was collected by step-scan modes in a θ–2θ range between 10° and 70° with step-size of 0.02° and step time of 0.6 s. Pure silicon (~99.9999 %) was used as an internal standard. The elemental composition of the films was analyzed by using energy dispersive X-ray spectrometer unit (EDXS) interfaced with a scanning electron microscope (SEM), (JOEL XL) operating with an accelerating voltage of 30 kV, which was used for studying the morphology of the film. The relative error of determining the indicated elements does not exceed 2%. Both of optical transmittance (T) and reflectance (R) for as-deposited CdI_2 thin films were measured as a function of wavelength by using a double beam (JASCO, V-670 UV–VIS–NIR) spectrophotometer. The light beam was normal incident on the glass substrate coated by CdI_2.

3. Result and discussion

3.1. Determination of the structure parameters of CdI_2 thin film

To investigate structure parameters characterizing crystallize size (D_v) and lattice strain (ε), the intensities were calculated by step scanning technique with small interval ($\Delta\theta = 0.02$). A period of 10 s was taken at each fixed value of 2θ leading to a reasonable number of counts. Fig. 1(a) shows the XRD spectra of CdI_2 powder, while Fig. 1(b) represents a simulate scan from the pattern according to Ref. Code 12-574 cards using X'Pert HighSore (version 1.0e) program.

The XRD patterns of CdI_2 films of various thicknesses deposited on glass substrates are shown in Fig. 2. The XRD analysis reveals that the films are polycrystalline of hexagonal structure with the peaks at $2\theta = 12.32°$, 26.033° and 53.413° is corresponding to (002), (004), and (008) orientations, respectively (JCPDS Data file: 00-012-0574-hexagonal). It can be seen that, the peak intensity increases with increasing film thickness. Each XRD line profile is broadened due to instrumental and structure factors, crystallite size (D_v) and lattice strains (ε) [15]. Therefore, the first indispensable preparatory step to calculate D_v and ε from the recorded

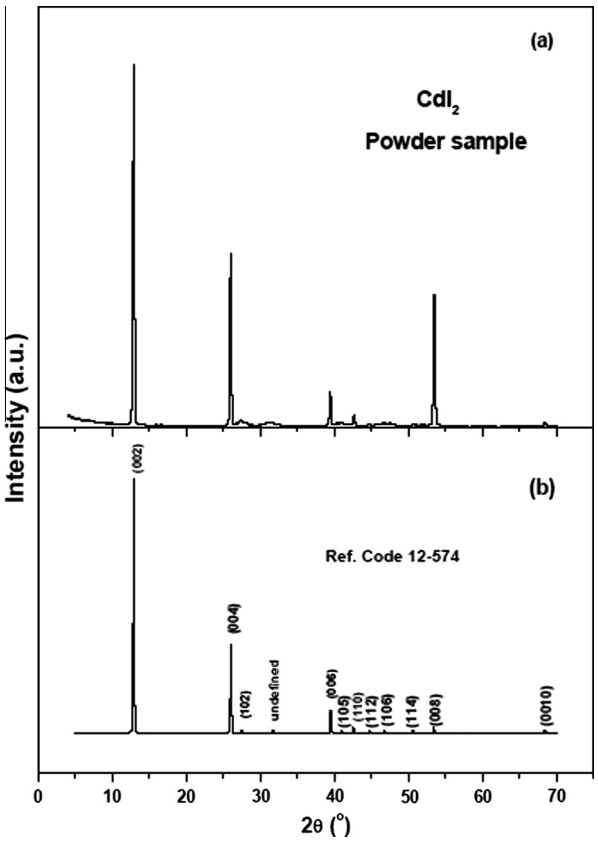

Fig. 1. (a) X-ray diffraction spectra of CdI_2 powder and (b) a simulate scan from pattern according to the Ref. Code 12–574 cards using X'Pert HighSore (version 1.0e) program.

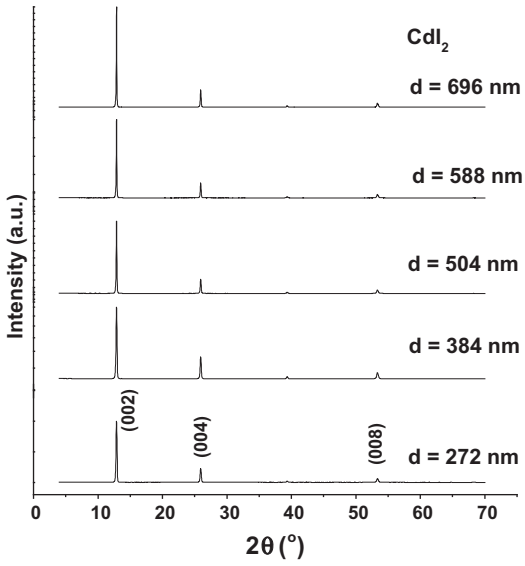

Fig. 2. XRD patterns of CdI_2 films of different thickness on glass substrates.

XRD scan is the determination of pure diffraction line profile for a given reflection whose integral breadth depends solely on the structure factor [15]. This pure line profile is extracted by deconvoluting the instrumental broadening factor from the experimental line profile. Then, only pure line profile can be used for calculating the D_v and ε. In the present work, both of D_v and ε can be obtained for the Voigt function and the integral breadth, which can be used to determine the fractional Lorenzian and Gaussian components in the convolution.

The under taken steps for determining structure parameters, namely, the crystallite size and micro strain, are in the following:

1. From the resulted ($I/2\theta$) spectrum, a considerable value of the background intensity have been considered, then, the corrected intensities (I_{corr}) were determined, and the value of the maximum intensity (I_o) has been obtained.
2. The summation of the corrected intensities have been calculated and denoted by $I_G = \sum I_{corr}$
3. The integrated breadth (β) of the reflection has been determined from the relation: β = (Area under the peak)/I_o or

$$\beta = \frac{(I_G \times \text{step interval}\,(0.02))}{I_0} \tag{1}$$

4. The Voigt function is determined from the relation

$$\phi = \frac{\text{FWHM}}{\text{integral breadth}\,\beta} \tag{2}$$

5. The obtained values from Voigt function and integral breadth were used to determine the fractional Lorenzian and Gaussian components in the convolution. Asthan and Kiefer [15] gave a simple expiration from which such fractional components could be evaluated by

$$\beta_L = \beta(a_0 + a_1\phi + a_2\phi^2) \tag{3}$$

$$\beta_G = \beta(b_1 + b_{1/2}[\phi - 2\pi] + b_1\phi + b_2\phi^2) \tag{4}$$

where $a_0 = 2.027$, $a_1 = -0.4803$, $a_2 = 1.7756$, $b_o = 0.4620$, $b_{1/2} = 1.4187$, $b_1 = -2.2043$ and $b_2 = 1.8706$. where β_L and β_G are the Lorentzian and Gaussian distributions, respectively.