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The influence of heat treatment on the crystallite size, dislocation density, stacking faults probability and optical band gap of nanostructured cadmium sulfide films

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ABSTRACT

Nanocrystalline cadmium sulfide films were deposited on the ordinary glass slide substrates by chemical bath deposition. Two advanced X-ray diffraction analyses i.e. DIFFaX and eCMWP were applied and the microstructure of films was evaluated as a function of annealing temperature. The optical properties of samples were also studied, using the transmittance spectra in the wavelength range of 300–900 nm. Based on our studies, we have found that with the elevation of annealing temperature, the crystallite size increases, however, the dislocation density, the fraction of stacking faults and the band gap energy decrease and the outer cut-off radius of dislocation does not appreciably change. We can also see that the energy gap follows the linear, inverse square and quadratic relation with uniform strain, crystallite size and dislocation density, respectively. Comparing the microstructure evaluated from eCMWP with the results of Scherrer formula and Williamson–Hall plot shows that there is no agreement between the results of advanced and early X-ray diffraction analysis.

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1. Introduction

Recently there has been growing interest in the study of nanoscopic metal chalcogenide semiconductors (MCS). Novel chemical and electrical properties together with nonlinear optical phenomena observed in these materials have led to their use in a variety of industries [1,2]. They have potential applications in the gas sensors [3], light emitting diodes [4], photocatalysts [5], solar cells [6,7] and optoelectronic devices [8]. The exclusive physical properties of MCS nanoparticles strongly depend on the shape, size and lattice defects [9].

So far several attempts have been made to evaluate the influence of microstructure on the physical properties of MCS materials. Most of the techniques used in these studies are limited to the data obtained from the scanning and transmission electron microscopy (TEM and SEM) [10,11], atomic force microscopy (AFM) [12,13] and the old X-ray diffraction analysis (Scherrer formula [14,15] and Williamson–Hall plot [16,17]). However, the defect density in crystalline nanomaterials is very high [18] and hence, in many cases, the resolution of electron microscopy images is not clear enough to detect the linear or planar defect. Also in these materials, ignoring the distortion broadening in Scherrer formula might yield incorrect results. According to the advanced theory of X-ray diffraction and its respective analysis, in most nanocrystals, the variation of integral breadth is not a monotonous function in terms of the diffraction vector [19–21]. For this case, which is

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referred to the anisotropic strain broadening [22], the Williamson–Hall plot cannot capture a correct microstructure. On the other hand, in some literature the inverse square of the crystallite size has been defined as the dislocation density appearing in crystals [23,24]. In this assumption the effects originating from the crystal systems (cubic, hexagonal, tetragonal, etc.), activity of slip systems and dislocation contrast factor as well as the influence of the Burgers vectors on the peak profile broadening are neglected. Therefore, it seems that in the study of the relation between the microstructure (in terms of crystallite size and lattice defects) and physical properties of MCS materials, the advanced XDA methods must be applied instead of the conventional approaches.

In the present work, the microstructure and optical properties of cadmium sulfide thin films were investigated. To do this, the peak profiles of faulted cadmium sulfide crystals are simulated at different fractions of stacking sequences using the DIFFaX software [25]. By making a comparison between the calculated profiles and measured X-ray diffraction data for the cadmium sulfide films, it is shown that the more pronounced effect of stacking fault is on the anisotropic line broadening. The results of DiFFaX software are incorporated into the eCMWP fitting procedure [26,27], the crystallite size, the dislocation density and the stacking faults of CdS films, which were annealed at the temperature interval [300–500 °C], have been quantitatively evaluated. The values of crystallite size and dislocation density derived from eCMWP are compared to those obtained from the Scherrer and Williamson–Hall methods. It is found that there is no meaningful connection between the early and advanced X-ray diffraction methods. Therefore, it appears that in the study of the relation between physical and microstructure properties, the advanced X-ray diffraction analysis must be applied instead of the old one. Finally the optical band gap of CdS films was calculated, using the optical transmission spectra of films and the influence of crystallite size, dislocation density and uniform strain on the energy gap of CdS films was evaluated.

2. Theoretical backgrounds

2.1. DIFFaX software

In this study the DiFFaX software was used to simulate the powder diffraction profiles of cadmium sulfide crystal containing planar defects. This software is based on the self-similarity of stacking sequence (which is presented in periodic objects and constructed by nondeterministic layer stacking) to calculate the direct intensity distribution. In mathematical language the scatter wave function, $\Psi(\mathbf{u})$, of each crystal centered on any layer can be expressed in terms of the scattering contribution of that layer $F(\mathbf{u})$ plus the scatter wave function of the displaced $\exp(-2\pi i\mathbf{u}\cdot\mathbf{R})\Psi(\mathbf{u})$ crystal, centered at the next layer [26]:

$$\Psi(\mathbf{u}) = F(\mathbf{u}) + \exp(-2\pi i\mathbf{u}\cdot\mathbf{R})\Psi(\mathbf{u}), \quad (1)$$

in which $\mathbf{u}$ and $\mathbf{R}$ are the reciprocal space vector and the shift between the origins of layer and the displaced crystal, respectively. Applying the recursive procedure, substituting the $\Psi(\mathbf{u}) = F(\mathbf{u})/(1-\exp(-2\pi i\mathbf{u}\cdot\mathbf{R}))$ into the above equation and extending this recursive property to the crystal containing planer defects, the scatter wave function of crystal can be obtained in the following form [28]:

$$\Psi_i(\mathbf{u}) = F_i(\mathbf{u}) + \sum_{j=1}^{N} \alpha_{ij}\exp(-2\pi i\mathbf{u}\cdot\mathbf{R}_{ij})\Psi_j(\mathbf{u}), \quad (2)$$

where i index corresponds to a specific layer type and α_{ij} is the transition probability from layer i to layer j. Both of the i and j layers go from 1 to N, where N is the number of type of layer. Now, supposing that the scattering is composed from the statistical ensembles of crystallites, so that the intensity of simulated profiles is the product of incoherent sum of intensities, scattered by the individual crystallites:

$$\frac{I(\mathbf{u})}{N} = \sum_{j=1}^{N} g_j\left[F^*(\mathbf{u})\Psi(\mathbf{u}) + F(\mathbf{u})\Psi^*(\mathbf{u}) - \left|F_j(\mathbf{u})^2\right|\right], \quad (3)$$

where g_j is the probability of layer type j occurred in a crystal and defined in the following form:

$$g_i = \sum_{j=1}^{N} g_j\alpha_{ij}, \quad \sum_{j=1}^{N} g_j = 1. \quad (4)$$

2.2. eCMWP fitting procedure

In order to evaluate the microstructure of CdS films in terms of crystallite size, size distribution, dislocation density and planar faults, we used the eCMWP procedure. In the algorithm of this software the observed peak profiles (I^O) are the convolution of instrumental (I^I), size (I^S), distortion (I^D) and planar defects (I^{PD}) profiles:

$$I^O = I^I \otimes I^S \otimes I^D \otimes I^{PD} + I^{BK}, \quad (5)$$

where I^{BK} is the background intensity. According to Warren–Averbach approach, the Fourier coefficients of $I^{SD} = I^S \otimes I^D$ are the multiplication of the size, $A^S(L)$, and distortion, $A^D(L)$, Fourier coefficients [29]:

$$\ln A^{SD}(L) = \ln A^S(L) + \ln A^D(L), \quad (6)$$

where L is the Fourier length. Assuming the shape of crystallites and the distribution of grains as spherical and lognormal functions, the Fourier size can be written in the following form [30]:

$$A^S(L) = \int_{|L|}^{\infty} (x^2 - |L|x)\,erfc\left[\frac{\log(x/m)}{\sqrt{2}\sigma}\right] dx, \quad (7)$$

where m and σ are the median and the variance of lognormal distribution respectively. Using m and σ in the following equation, the volume weighted average crystallite size is determined [31]:

$$\langle D_V \rangle = 3/4m\exp(3.5\sigma^2). \quad (8)$$

In dislocated poly-crystalline materials, the main source of strain anisotropy is the dislocation and the second term on the right-hand side of Eq. (6) is as follows [32]:

$$A^D(L) = \exp\left[-\frac{\pi}{2}(gL)^2\rho\overline{Cb^2}f\left(\frac{L}{R_e}\right)\right], \quad (9)$$

where g, ρ, $f(L/R_e)$ and R_e are the diffraction vector, dislocation density, Wilkens function and outer cut-off radius of dislocation, respectively. $\overline{Cb^2}$ is the average

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