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# Structural characterization and optical properties of ZnSe thin films

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**Abstract**

Zinc selenide (ZnSe) thin films ($d$ = 0.11–0.93 μm) were deposited onto glass substrates by the quasi-closed volume technique under vacuum. Their structural characteristics were studied by X-ray diffraction (XRD) and atomic force microscopy (AFM). The experiments showed that the films are polycrystalline and have a zinc blende (cubic) structure. The film crystallites are preferentially oriented with the (1 1 1) planes parallel to the substrate surface. AFM images showed that the films have a grain like surface morphology. The average roughness, $R_a$ = 3.3–6.4 nm, and the root mean square roughness, $R_{rms}$ = 5.4–11.9 nm, were calculated and found to depend on the film thickness and post-deposition heat treatment.

The spectral dependence of the absorption coefficient was determined from transmission spectra, in the range 300–1400 nm.

The values of optical bandgap were calculated from the absorption spectra, $E_g$ = 2.6–2.7 eV.

The effect of the deposition conditions and post-deposition heat treatment on the structural and optical characteristics was investigated.
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## 1. Introduction

In recent years, the study of the electronic transport and optical properties of the zinc selenide (ZnSe) required a considerable attention because this compound offers an important number of applications in optoelectronic device technologies (photodetectors, solar cells, blue light-emitting diodes, etc.) [1–4].

ZnSe thin films have been prepared by various techniques such as thermal evaporation under vacuum, molecular beam epitaxy, organo-metallic chemical vapor deposition, solution growth, spray pyrolysis, etc. [5–8]. It was established that structural, electrical and optical properties of these films are very sensitive to deposition conditions and post-deposition heat treatments [9–11].

In the previous papers [9–11], we showed that the mechanism of electronic transport in polycrystalline ZnSe thin films can be explained by applying the Seto's model [12] with several modifications proposed by Baccarani et al. [13]. Some optical properties of ZnSe thin films have been studied in [10].

In the present paper, we extended these investigations by studying the effect of the post-deposition heat treatment on the structural characteristics and optical properties (transmission and absorption spectra, dispersion of refractive index) of ZnSe thin films prepared by quasi-closed volume technique, under vacuum.

## 2. Experimental

ZnSe thin films were deposited onto glass substrates by vacuum evaporation of high-purity (99.999%) ZnSe polycrystalline powder. The quasi-closed volume technique was used [14]. Deposition arrangement has been described in detail in [9,10,14].

The experimental arrangement permitted us to prepare the films under following conditions: the deposition rate, $r_d$, ranged between 0.15 nm/s and 2.59 nm/s; source–substrate distance was about 8 cm; substrate temperature, $T_s$, was 300 K; the temperature of evaporation source, $T_{ev}$, was 1070 K.

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The film thickness was determined by an interferometric method (multiple-beam Fizeau's fringe method [15]) and, for studied samples, ranged between 0.11 μm and 0.93 μm.

The film crystalline structure was examined by X-ray diffraction (XRD) technique, with a DRON-2 diffractometer (using $CoK_{\alpha}$ radiation). The surface morphology was studied by atomic force microscopy (AFM).

For heat treatment of films, the following succession of technological runs was used: a heating from room temperature to an annealing temperature ($T_a$ = 500 K); an annealing for a certain time ($t_a$ = 0–60 min) at determined temperature, $T_a$ and, finally, a cooling from annealing temperature to the room temperature [9,16,17]. In all cases the temperature rate was about 5 K/min.

Reflection and transmission spectra, in the spectral domain 300–1400 nm, were recorded (at room temperature) using a PMQII (C. Zeiss, Jena) double beam spectrophotometer and an ETA-STC (EtaOPTIK Steag) spectrometer [16,17].

## 3. Results and discussion

The XRD patterns indicate that the samples, obtained from described procedure, are polycrystalline and have a cubic (zinc blende) structure.

Figs. 1–3 show XRD patterns for some ZnSe films deposited in different conditions. The Miller indices, (h k l), are indicated on each diffraction peak. For all samples a major peak is seen at about 31.7° and equivalent inter-planar spacing of 3.275 Å corresponds to (1 1 1) plane reflections from cubic type zinc blende. This fact indicates that the film crystallites are preferentially oriented with (1 1 1) planes parallel to the substrate. Other peaks, except cubic ZnSe are not identified in the XRD patterns.

After heat treatment, the film structure is improved and the orientation degree of crystallites increases (an increase of peak intensities corresponding to (1 1 1) planes of ZnSe take place) (Figs. 2 and 3). The presence of an amorphous phase is also evidenced by XRD patterns [18].

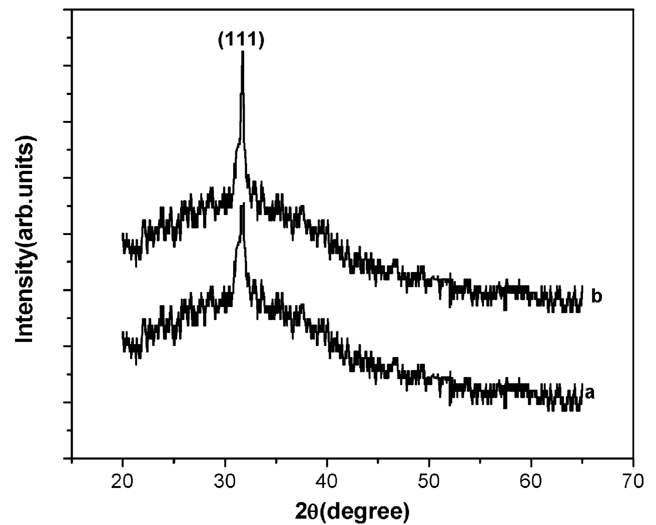


Fig. 2. Effect of the heat treatment on the XRD patterns for ZnSe thin films (substrate temperature, $T_s$ = 300K; deposition rate, $r_d$ = 1.33 nm/s; film thickness, $d$ = 0.490 μm); (a) before heat treatment, (b) after heat treatment (annealing temperature, $T_a$ = 500 K; annealing time, $t_a$ = 60 min).

The crystallite size, $D$, has been determined using the Debye-Scherrer formula [18]

$$D = \frac{k\lambda}{\beta_{2\theta}\cos\theta}, \quad (1)$$

where $k$ is the Scherrer's constant ($k$ = 0.90 [18–20]), λ denotes the wavelength of X radiation, $\beta_{2\theta}$ is the full-width at half-maximum and $\theta$ is the Bragg angle.

The values of some structural parameters, determined from XRD patterns, are indicated in Table 1.

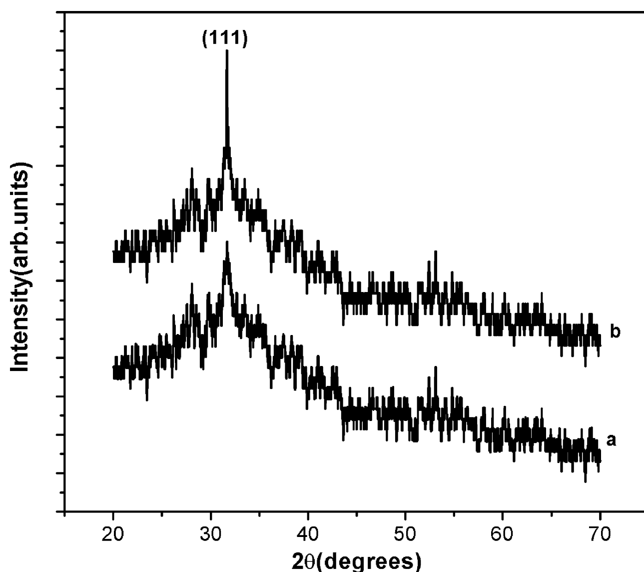


Fig. 1. XRD patterns for ZnSe thin films prepared at substrate temperature $T_s$ = 300 K. Deposition rate: (a) $r_d$ = 0.11 nm/s; (b) $r_d$ = 0.70 nm/s. Film thickness: (a) $d$ = 0.13 μm; (b) $d$ = 0.30 μm.

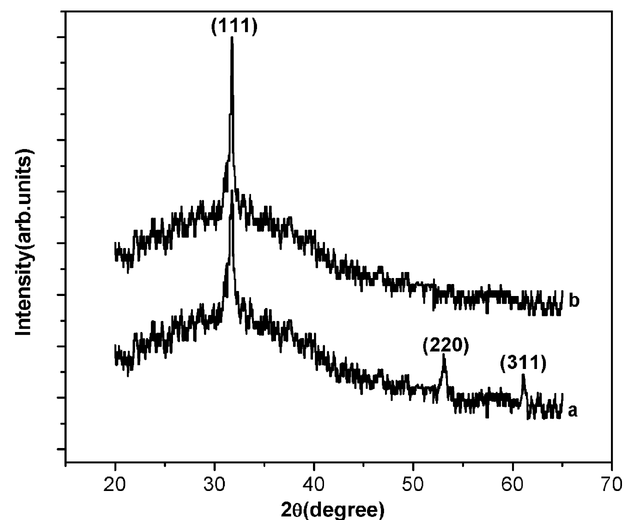


Fig. 3. XRD patterns for as deposited (a) and heat treated (b) ZnSe thin films. Deposition conditions: substrate temperature, $T_s$ = 300 K; deposition rate, $r_d$ = 1.29 nm/s; film thickness, $d$ = 0.850 μm (annealing temperature $T_a$ = 500 K; annealing time, $t_a$ = 60min).

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