Synthesis and characterization by experimental and theory research suitable on the CdS and CdO materials

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Abstract. In this paper, we have compared and analyzed experimental and theoretical research on \( \text{CdS} \) and \( \text{CdO} \) types semiconductor materials. The XRD spectra of the samples were examined using an atomic force microscope and X-ray diffraction microscopy. During film deposition, the temperature of the crucible with a source (CdS) varied in the range \( T_{\text{source}} \approx 800 \div 850 \) °C, and the substrate temperature was maintained within the range \( T_{\text{substrate}} \approx 250 \div 270 \) °C. In this case, to ensure the reproducibility of the structures, a shutter was used, with the help of which the CdS deposition time was set, which ensured that the film thickness was the same from experiment to experiment.

1 Introduction

Cadmium sulfide is a dye from strong yellow to dark red. Cadmium sulfide was first synthesized in Germany in 1817 and then sold to artists as a pigment in the mid-19th century. However, its use did not become widespread until about 1917. Finely dispersed, stable, light-resistant particles have a deep color. Initial preparations of cadmium pigments had different particle sizes ranging from 0.1 to 7 micrometers, while recently obtained pigments contained only submicron particles [1]. CdS and CdO films are used as electrodes in liquid crystal displays, photodiodes, and other devices. There are few well-known wide-gap compounds and oxides that conduct currents [2-4]. Zinc oxide (\( \text{ZnO} \)), indium oxide (\( \text{In}_2\text{O}_3 \)) and tin oxide (\( \text{SnO}_2 \)) are the most widely known. The optical band gaps of these materials are \( \text{E}_g > 3 \text{eV} \) and they all have \( \text{n-type} \) conductivity. It is difficult to obtain ZnO films, and in order to obtain a low-resistance (\( \text{In}_2\text{O}_3 \)) film, it is necessary to grow it at a temperature of about 400°C or carry out subsequent annealing [5]. This is not always.
2 Experimental technique and results
There is a certain “critical” temperature at which changes in the nucleation process are observed, above which it is difficult to obtain a high-quality film that completely and evenly covers the substrate. Therefore, to obtain high-quality films, the deposition of the latter is carried out below the critical temperature ($T_{cr}$), but close to it. At the same time, in order to avoid contamination of the deposited film with impurities located on the surface of the evaporated substance, as well as to bring the temperature of the evaporator to operating conditions, before the start of evaporation, the substrate surfaces are protected by a damper, which temporarily blocks the flow of evaporated atoms and molecules towards the substrate during heating. The film deposition rate is directly proportional to the evaporation rate. The flux of atoms or molecules condensing on the substrate surface at fixed temperatures of the evaporator and substrate is determined by the expression \[ N_p = k \frac{A}{l^2} N_i \] (1)

Where $N_i$ is the flux of evaporating particles; $l$ is the distance from the source to the substrate; $A$ is the coefficient taking into account the shape and molecular-kinetic characteristics of the evaporator; $k$ - condensation coefficient - the ratio of the number of molecules condensed on the surface of the substrate to the number of molecules that hit the surface of the substrate, numerically equal to the ratio of the rate of condensation and the rate of evaporation.

Almost always, evaporation is carried out at temperatures exceeding the evaporation temperature of the substance (forced mode) in order to ensure sufficiently high vaporization rates and thereby reduce the effect of residual gases on the properties of the deposited films. At low evaporation rates, the formation of loose, rough films is possible.

The thickness of the deposited film is set by controlling the deposition time ($t_{sp}$). When a predetermined value of the film thickness is reached, the flow of atoms or molecules of the substance is blocked by a damper and, at this, the film growth stops. In this case, depending on the technological process, heating of the substrate can continue or stop. During the entire technological process, a vacuum of the order of $10^{-5}$ Pa is constantly maintained in the chamber.

To heat the evaporated substance to a temperature at which it begins to evaporate intensively, various methods are used. Basically, heating is carried out by an electron flow, laser, concentrated solar or microwave radiation, using resistive heaters, etc. In general, the vacuum deposition method is very diverse both in terms of heating the evaporated substance and in the design of evaporators. In the case when it is required to obtain films from multicomponent substances, then in this case several evaporators are used. Since the evaporation rate of different materials is different, it is rather difficult to ensure the reproducibility of the chemical composition of multicomponent films obtained by vacuum deposition. Therefore, the thermal vacuum spraying method is mainly used for single-component pure materials.

Obtaining thin films using vacuum deposition is the most interesting from the point of view of practical application, as based on them, you can create a variety of photosensitive structures with a high speed due to the small minority carrier lifetime. Studies of the crystal structure of the CdS films obtained by us by this method showed the presence of both cubic ($\beta$), and hexagonal ($\alpha$) modifications. In [9] it was shown that the hexagonal phase is increased by the annealing. The transition hexagonal $\rightarrow$ cubic as a result of the elevated temperature of the substrate is observed in films up to 0.4 µm thick; at large thicknesses, mixed phases followed by an increase in the hexagonal phase and the disappearance of the cubic phase. The transformation depends on the growth rate. For its implementation, small growth rates are required.

All investigated CdS films were obtained by the method described above, i.e., by thermal spraying of powders of the binary compound CdS (semiconductor purity). CdS was
deposited slowly, as described in [10] in a quasi-closed vacuum system with a residual pressure of $10^{-5}$ Torr. Glass was used as substrates. However, all the same, the contaminants present on the surface of the substrates, formed as a result of long-term storage, require their removal from the surface of the substrate and its refreshment. For this purpose, we used washing, which was carried out by the displacement method [11] in two stages: first, the substrates were washed with running distilled water for 8–10 minutes, then with deionized water for 3–5 minutes. After that, the substrates were dried in an oven with infrared drying for 15–20 minutes. During film deposition, the temperature of the crucible with a source (CdS) varied in the range $T_{\text{source}} \approx 800 \div 850 \degree$ С, and the substrate temperature $T_{\text{p}} \approx 250 \div 270 \degree$ С. In this case, to ensure the reproducibility of the structures, a shutter was used, with the help of which the CdS deposition time was set, which ensured that the film thickness was the same from experiment to experiment. The resulting films had a thickness $w \approx 400$ nm, and an $n$-type conductivity with a resistivity $\rho = 200 \, \Omega \, \text{cm}$. Next, the morphology of CdO and CdS films was studied (Figs. 1a) and 2a). And in fig. 1 b) and 2 b) show X-ray diffraction analysis of CdO and CdS films. From the film morphology, the crystallite size was determined, which was about 50 nm for CdO films, and about 100 nm for CdS. The surface morphology of thin films was tested using an atomic force microscope (AFM) (hpAFM, Nano Magnetics). The XRD spectra of the samples were examined using an atomic force microscope and X-ray diffraction microscopy. Here we present our results as an AFM micrograph and XRD plot.

Fig. 1. (a) Micrograph of thin CdO films deposited by atomic layer deposition. (b) Wide-angle X-ray spectra of thin CdO films.

Fig. 2. (a) Micrograph of thin CdS films obtained by atomic layer coating. (b) Wide-angle emission spectra of thin CdS films.
Figure 3 shows the absorption spectra of the thin films of CdO and CdS. The optical absorption of thin films was analyzed by fiber spectrometer (HR4000, Ocean Optics). These measurements allow estimating optical band gaps of the transparent thin films deposited on the surfaces of the glass substrates.

**3 Analytic solutions**

\[ I_\nu(x) = I_{\nu 0} (1 - R_\nu) \exp(-ax) \]

\[ \alpha(\nu) = -\frac{\partial I_\nu(x)}{\partial x} \]

\[ \alpha(\nu) = -\frac{N(\nu) \cdot \nu}{I_{\nu 0}} \]

\[ N(\nu) = \frac{2}{(2\pi)^3} \int d^3k_j \int W_{fj} \left[ f(k_f) - f(k_j) \right] d^3k_j \]

\[ k_f, k_j \rightarrow f(k_f), f(k_j) \]

\[ E_C \rightarrow E_V \rightarrow \alpha(\nu) \]

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**Fig. 3.** Absorption spectra of thin films, which were deposited by using atomic layer deposition method: (a) CdO thin film. (b) CdS thin film.
Fig. 4. Shows the dependence of the absorption coefficient of the CdS material on the photon energy according to the Tauc's model. To determine the expression $\alpha(h\nu)$, the energy of optical transitions is written as follows.

$$h\nu = E_g \pm \frac{h^2k^2}{2m^*}$$

where $m^*$ is the effective mass, $E_g$ is the bandwidth of the forbidden field (5) and (6) can be solved together by substituting (4) into expression (7). We obtain the following expressions (7) for allowed and forbidden transitions.

$$\alpha(h\nu) = A_1 \left(\frac{h\nu}{E_g}\right)^{1/2}$$

$$\alpha(h\nu) = A_1 \left(\frac{h\nu}{E_g}\right)^{3/2}$$

$A_1, A_2$ - Coefficients that do not depend on the frequency but include the parameters of the zones involved in optical transitions and some international constants.

4 Conclusions

In the transitions that occur with the release or absorption of a photon, we can see that the electron passes from the initial valence band $E_j, \text{and} k_j$ to the transient state $E_f, \text{and} k_f$ under the action of the photon, which can be considered as a two-step process. We can see that the coefficients $A_1, A_2$ also depend on the concentration of ionized acceptors in some semiconductors. From the film morphology, the crystallite size was determined, which was about 50 nm for CdO films, and about 100 nm for CdS. The surface morphology of thin films was tested using an atomic force microscope (AFM, hpAFM, E3S Web of Conferences 410, 02057 (2023))
Nano Magnetics). The XRD spectra of the samples were examined using an atomic force microscope and X-ray diffraction microscopy.

References


