Investigation of HgSe Films, Deposited from Aqueous Solutions with Different Complexing Agents

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Abstract – The process of synthesis of mercury selenide (HgSe) thin films by a chemical bath deposition method (CBD) with using different complexing agents (potassium rodanide, potassium iodide and sodium thiosulfate) has been investigated. The phase composition, crystal structure, absorption spectra, surface morphology of HgSe films were studied. The effect of nature of complexing agent on the properties of obtaining coatings was shown. The HgSe films have a sphalerite structure, nearly stoichiometric atomic ratios of mercury to selenium and optical band gaps, which are localized in the ranges 1.38-2.40 eV, depending on the usage of complexing agent.

Key words – mercury selenide, semiconductor films, chemical bath deposition, optical band gap, structure and morphology of thin films.

I. Introduction

Mercury selenide (HgSe) belongs to AIIIBVI group materials. The mercury chalcogenides can be used in in IR detectors, ultrasonic and gas sensors, catalysts, electrostatic reflective materials and solar cells [1-3].

Also there is great interest in the physical properties of nanometer size semiconductor films, because their properties are often superior to those of conventional coarse-grained polycrystalline materials [4].

Development of chemical synthesis of HgSe films with different complexing agents will allow to study the effects of the ligand nature on the properties of coatings. It will provide new possibilities for wave function engineering and in tailoring optical and optoelectronic properties of semiconductor films.

II. Experimental

The obtaining of HgSe semiconductor films is carried out by many methods. Technologically convenient way to their obtaining is by the method of chemical bath deposition (CBD) [5]. Compared with the other it allows to pursue the deposition at temperatures below 100°C on the large-sized substrates of different nature and use different combinations of starting substances.

The CBD of thin films of HgSe was conducted with the initial working solution which consisted of mercury nitrate (Hg(NO₃)₂), complexing agent, sodium selenosulphate (Na₂SeSO₄) and, if necessary, the pH-regulator. As complexing agents for mercury were used: potassium rodanide (KSCN), potassium iodide (KI) and sodium thiosulfate (Na₂S₂O₃); the pH-regulator – tri-

sodium citrate (Na₃C₆H₅O₇). The concentration of the Hg(NO₃)₂ solutions was equal to 0.05 M; KSCN – 2.0 M; KI – 0.1 M; Na₂S₂O₃ – 1.0 M; Na₂SeSO₄ – 0.25 M; Na₂C₆H₅O₇ – 1.0 M. Only freshly prepared reagents entered the working solutions for synthesis of HgSe films. The deposition duration and temperature of HgSe films, was 80 min and 20°C (in the case of using KSCN), 10 min and 90°C (in the case of using KI), 220 min and 20°C (in the case of using Na₂S₂O₃). The pH-regulator was added only at presence of sodium thiosulfate, because it was necessary to prevent its decomposition with formation of the sulfur. The chemical deposition has carried out on pre-prepared glass substrates with an area of 3.24 cm². After the end of the reaction the substrates were eliminated; the surface was cleaned with a distilled water to take off the remains of working solution and dried in air.

The phase composition of the HgSe films was investigated by X-ray powder diffraction (diffractometer DRON-3.0, CuKα radiation). Primary processing of the experimental diffraction data in order to identify the phases was made using the PowderCell program [6]. Optimum exposure for each of the samples was selected. Calculation of the cell parameters were done by using the FullProf software package [7]. The investigation of surface morphology of the films was carried out using a raster electron microscope REM-106Y equipped with a system for microanalysis. Absorption optical spectra of HgSe films were obtained with a spectrophotometer XION 500 (Dr.Lange). A comparative signal was passed through glass substrates identical to the substrates, used for the investigated films.

III. Results and discussion

The X-ray analysis of HgSe films has been held. It showed that films are single phase. Peaks that corresponded to the cubic phase of HgSe (sphalerite) (Fig. 1) can be identified on all diffractograms. The lines showed that films are single phase. Peaks that corresponded to the cubic phase of HgSe (sphalerite) (Fig. 1) can be identified on all diffractograms. The lines corresponding to the sulfur. The chemical deposition has carried out on pre-prepared glass substrates with an area of 3.24 cm². After the end of the reaction the substrates were eliminated; the surface was cleaned with a distilled water to take off the remains of working solution and dried in air.

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![Fig. 1. X-ray diffractograms of HgSe films, deposited with using different complexing agents: 1 – KSCN, 2 – KI, 3 – Na₂S₂O₃.](https://example.com/image-url)
The optical absorption spectra $A(\lambda)$ of HgSe films were investigated for wavelengths from 340 to 900 nm (Fig. 2). The HgSe films, deposited with using Na$_2$S$_2$O$_3$, has the biggest light absorption. Using KI makes this value averages. The lowest absorption of HgSe films was observed with use of KSCN. The decrease of the light absorption can be seen in all cases near 400 nm wavelengths region, which corresponds to mercury selenide and confirms the results of the phase analysis by X-ray diffraction. The spectral dependences in $(\alpha \cdot h\nu)^2$ vs. $h\nu$ coordinates allow determining the fundamental absorption edges. The optical band gaps of the films are localized in the ranges 1.38-2.40 eV, depending on the usage of complexing agent. These values corresponds to the literary data [8-10].

![Image](image.png)

**Fig. 2.** The spectral dependences of optical absorption of HgSe films, deposited with using different complexing agents: 1 – KSCN, 2 – KI, 3 – Na$_2$S$_2$O$_3$ (inset – $(\alpha \cdot h\nu)^2$ vs. $h\nu$ dependense)

Investigation of HgSe surface morphology at x5000 magnification (Fig. 3) showed that the films are homogeneous and solid, with small amounts of surface defects. The spherical particles are seen on the surface of the film at the case of using potassium rodanide.

![Image](image.png)

**Fig. 3.** Surface morphology of HgSe films, deposited with using different complexing agents: 1 – KSCN, 2 – KI, 3 – Na$_2$S$_2$O$_3$

The microanalysis of the surface of the HgSe films shows nearly stoichiometric atomic ratios of mercury to selenium with a slight excess of mercury atoms (at using of potassium iodide) or a slight excess of selenium atoms (at using of potassium rodanide and sodium thiosulfate).

**Conclusion**

The HgSe thin films were synthesized by the CBD method. The possibility of using different complexing agents was shown. The phase composition of obtained HgSe samples was determined. The optical absorption spectra, surface morphology of HgSe films were investigated. According to the results of microanalysis the elemental composition of coatings were studied. From the obtained data, the most suitable complexing reagent can be selected. The positive research results of obtained HgSe films allows to assuming that the chemical bath deposition method can be used to produce optical materials based on this coatings.

**Acknowledgement**

This research is under the project “Thin Film Semiconductor Materials for Photo Sensitive Solar Cells” (State Registration № 0117U004455).

**References**


