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# Mathematical approaches to a method of semiconductor materials films synthesis type $A^{II}B^{VI}$ for photosensitive structures used in alternative energy

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*Abstract*: The scientific direction of the synthesis of CdS and CdSe thin films by the method of chemical surface deposition (CSD) using the aqueous solutions of cadmium-containing salts: chloride, nitrate, sulphate, acetate and iodide has been developed. A mathematical model of the CSD process of CdS and CdSe thin films was developed to improve the efficiency of experiments and reduce costs. The model makes it possible to determine the concentration of reagents, the duration, and the CSD temperature, which are necessary to obtain films of a specified thickness. The optimization of chemical deposition parameters of film-type semiconductor materials has been carried out. Based on the mathematical model, the optimal synthesis conditions were the following: the concentration of cadmium-source salt – 0.01 mol/L, chalcogenizer – 1.0 mol/L or 0.1 mol/L in the case of thiourea or sodium selenosulphate, respectively; the temperature: 70 °C and the duration of 3 min. The mathematical dependence of the experimental studies results of the metal ions content in thin-film solar cells for the effective direct conversion of solar radiation into electrical energy was proposed taking errors into account.

*Keywords*: thin films; chemical surface deposition; solar cells.

## INTRODUCTION

Now in the public consciousness, there is a growing conviction that the energy of the future should be based on the large-scale use of solar energy, and in its various manifestations. The bet on solar energy should be seen not only as a win-win situation, but in the long term as one of the best choices for humanity. We will consider the possibilities of converting solar energy into electrical energy using semiconductor solar photocells in retrospective and prospective terms. These devices appear to be quite mature scientifically and technologically today to be

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regarded as the technical basis for the large-scale solar power of the future. Photovoltaic converters of solar energy occupy a special place among the alternative and the renewable energy sources.

Solar PV cells are a very real technically and cost-effective alternative to fossil fuels in several applications. The solar cell can directly convert solar radiation into electricity without the use of any moving mechanisms. Due to this, the service life of solar generators is quite long. Photovoltaic systems have proven themselves well since the beginning of the industrial application of photovoltaic cells.

Improving the photoconversion efficiency by increasing the short-circuit current in solar cells with a CdS or CdSe buffer layer requires a decrease in losses because of the optical absorption of photons with energies $h\nu < 2.4$ eV, which can be achieved by minimizing the thickness of cadmium sulphide and cadmium selenide films to optimal sizes. Therefore, the studies of the deposition process of CdS and CdSe thin films with the given photoelectric properties for the creation based on them of thin-film solar cells are of considerable practical interest.

The search for new approaches to obtain the films of $A^{II}B^{VI}$ semiconductor materials, in particular CdS and CdSe films, will solve the problems of reducing the cost of photosensitive elements, a comprehensive study of the electrophysical properties of film-type semiconductor materials and the structures based on them, as well as the development of new methods for their implementation. The prospect of this direction is justified by the fact that, despite numerous studies, semiconductor photosensitive structures based on cadmium sulphide and cadmium selenide thin films are widely used in thin-film solar cells for the efficient direct conversion of solar radiation into electrical energy.[1,2] The industrial introduction of such elements and the use of solar modules in alternative energy is hindered by the high cost of their manufacture, and, accordingly, the high cost of electricity produced by them. The manufacturing cost can be significantly reduced if the method for obtaining thin films is simple and will not require the use of high temperatures and expensive initial materials.

The operation of thin-film elements is based on a Cd (S, Se)/CdTe or Cd (S, Se)/Si heterojunction, and their parameters and technical characteristics are determined by the properties of thin films and the conditions for making the heterojunctions. Therefore, the development of the synthesis basis of CdS and CdSe continuous semiconductor thin films from aqueous solutions using a simple and reproducible method that must satisfy the economic and environmental aspects of production and must ensure high quality of the material is an important and actual scientific problem.[3] The use of mathematical modelling for the decrease of the film manufacturing cost and the increase of its production amount was not observed in the scientific research in this field, which can open a new approach to economical, and environmentally friendlier semiconductor synthesis in terms of decreasing the amount of by-products formation and the increase of the effectiveness of reactants conversion.

To obtain a high-quality mathematical model, it is essential to gather a substantial amount of experimental data related to the nature of the initial agents, concentration, synthesis temperature and duration, as well as film thickness.

To acquire this data, the following steps are necessary:

1. Choose the synthesis technique, initial substances, and synthesis conditions.
2. Produce several thin film samples.
3. Determine their thickness, optical, and morphological properties.
4. Establish relationships between these properties.

*Chemical surface deposition (CSD)*

To achieve the goals of this research, first of all, it was necessary to choose the film synthesis technique because the number of factors which should be used for the mathematical modelling and the quality of the film directly depends on the process which lay in its base. For this reason, we decided to use the chemical surface deposition technique since it requires the minimum amount of reactants, and this method is ideal for the production of thin films over large areas at temperatures <100 °C, which is one of the main requirements for the mass use of solar energy. The technology of chemical deposition of semiconductor films consists of the deposition of a solution containing metal ions and a source of sulphur or selenium ions onto a substrate. The deposition of CdS thin films from aqueous solutions is a reaction between cadmium salts and thiourea in an alkaline medium.[4,5] To obtain high-quality cadmium coatings, it is necessary to use well-water-soluble cadmium sources, which will be cheap and would not provide any additions, which may cause the formation of other undesirable by-products. For this purpose, it perfectly fits some simple cadmium salts. Preferably, the most used are $CdSO_4$, $CdI_2$, $Cd(NO_3)_2$, $Cd(CH_3COO)_2$ and $CdCl_2$. Thiourea is used as a sulphur-containing agent in the sulphide deposition reactions since it has a high affinity for metal cations and decomposes at low temperatures. The deposition process can be described by two mechanisms: homogeneous and heterogeneous.[6]

The homogeneous mechanism presupposes the formation of a coating of colloidal CdS particles, which are formed in solution and consist of several stages:

1. Dissociation of ammonium hydroxide:

$$NH_4^+ + OH^- \rightarrow NH_3 + H_2O \quad (1)$$

In an alkaline medium due to the interaction of $Cd^{2+}$ with $OH^-$ is the possible formation of an undesirable product – $Cd(OH)_2$:[4,5]

$$Cd^{2+} + 2OH^- \rightarrow Cd(OH)_2 \downarrow \quad (2)$$

2. Hydrolysis of thiourea, $(NH_2)_2CS$, with the formation of sulphides:

$$(NH_2)_2CS + H_2O \rightarrow HS^- + H^+ + (NH_2)_2CO \quad (3)$$

$$HS^- + OH^- \rightarrow S^{2-} + H_2O \quad (4)$$

3. Formation of the final product:

$$Cd^{2+} + S^{2-} \rightarrow CdS\downarrow \quad (5)$$

According to the heterogeneous mechanism of CdS thin films, the deposition from aqueous solutions passes through the stage of $[Cd(NH_3)_4]^{2+}$ formation, which reduces the overall reaction rate and prevents the formation of $Cd(OH)_2$.[7] The formed cadmium tetraamine ion interacts with sulphides, which are formed by hydrolysis of thiourea (Eqs. (3) and (4)):

$$Cd^{2+} + 4NH_4OH \rightarrow Cd[(NH_3)_4]^{2+} + 4H_2O \quad (6)$$

$$Cd[(NH_3)_4]^{2+} + S^{2-} \rightarrow CdS\downarrow + 4NH_3 \quad (7)$$

In general:

$$Cd[(NH_3)_4]^{2+} + (NH_2)_2CS + OH^- \rightarrow CdS\downarrow + 4NH_3 + H^+ + (NH_2)_2CO \quad (8)$$

The deposition of sulphide films from thiourea coordination compounds has several chemical features.

Depending on the salt nature and the composition of the solution different coordination forms may dominate, moreover together with the thiourea molecules the anions $Cl^-$, $Br^-$ and $I^-$ may enter the complex inner sphere under certain conditions with $SO_4^{2-}$. Thus, the nearest environment of cadmium atoms can be sulphur, halogen and oxygen atoms, moreover, during thermal destruction, some of the Cd–Hal or Cd–O bonds are stored and defects $Hal_S^{\bullet}$ and $O_S^{\bullet}$ are formed in the sulphide lattice.[8]

The orientation of thiourea complexes occurs on the active centres of its surface at the interaction with the substrate. Complex particles capable of interacting with the active centres of the substrate are the link that provides the binding of sulphide to the substrate. The nature of this interaction also determines the nature of film adhesion.

In the case of cadmium sulphide deposition on quartz or glass substrates, the active centres are silanol groups (≡Si–OH), which interact with halide or hydroxyl mixed complexes. As a result of this interaction, the oxygen bridges of the Cd–O–Si type are formed.[9] This explains the good adhesion of cadmium sulphide films obtained from thiourea coordination compounds to glass substrates.

CSD technology allows to obtain of thin films by using the sample surface as a heat source. The surface tension of the solution ensures that the volume of liquid used is minimized. The combination of the heat delivery method to the surface and a small volume of the solution leads to the high utilization of cadmium and its compounds.

Summarizing the above it can be argued that due to the several disadvantages of the described methods for obtaining compounds of the $A^{II}B^{VI}$ group, the search for more efficient, cost-effective technologies is relevant. In this aspect, the CSD method of thin semiconductor films is of considerable interest. This is indicated by numerous publications and research studies conducted by us.

The process of chemical surface deposition was carried out at room temperature by dosed application of the working solution on a pre-prepared surface of an optically homogeneous glass plate (18 mm×22 mm). The plates with the working solution were placed on a preliminarily thermostated surface to ensure uniform heating. The surface tension of the solution ensures that the volume of the reaction mixture is minimized and its retention on the substrate at the CSD method.

The film deposition occurs by heterogeneous nucleation of the compound on the substrate surface during heat transfer to the solution (Fig. 1). The heterogeneous nucleation is preferred over homogeneous fallout due to the thermal stimulation of chemical activity on a warmer growth surface. As a result, a high proportion of cadmium from the solution in the film is obtained and it depends on the substrate heteroepitaxial growth of the film. The heat outflow from the solution to the environment helps to maintain favourable conditions for the heterogeneous growth of the film over the period required for the film deposition. After heating the glass plate was taken away, and the surface was washed with a stream of distilled water and dried in air.

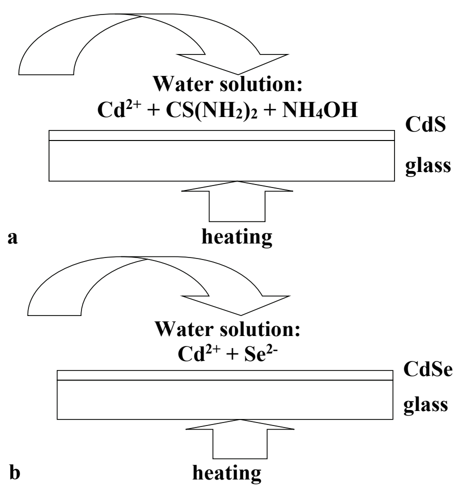


Fig. 1. The scheme of obtaining thin films (a – CdS; b – CdSe).

The freshly prepared aqueous solutions of cadmium salts were used to obtain CdS and CdSe thin films by CSD: $Cd(CH_3COO)_2$, $CdSO_4$, $CdCl_2$, $Cd(NO_3)_2$,

$CdI_2$. The solutions composition and the corresponding concentrations are given in Tables I and II.

TABLE I. Composition and solutions concentrations for CdS films

| Salt | $c$(cadmium salt) mol/L | $c(CS(NH_2)_2)$ mol/L | $c(NH_4OH)$ mol/L | Temperature °C |
|---|---|---|---|---|
| $Cd(CH_3COO)_2$<br>$CdCl_2$<br>$CdI_2$<br>$CdSO_4$<br>$Cd(NO_3)_2$ | 0.01–0.05 | 0.5–1.5 | 1.8 | 50.0–90.0 |

TABLE II. Composition and solutions concentrations for CdSe films

| Salt | $c$(cadmium salt) mol/L | $c(Na_2SeSO_3)$ mol/L | Temperature °C |
|---|---|---|---|
| $Cd(CH_3COO)_2$<br>$CdCl_2$<br>$CdI_2$<br>$CdSO_4$<br>$Cd(NO_3)_2$ | 0.01–0.05 | 0.1–0.4 | 50.0–90.0 |

CSD allows to obtain the films with structural, optical and electrical parameters that are not inferior to the films prepared by other methods. Also, CSD makes it possible to control film growth, maintain accurate process parameters, and dynamically change conditions to obtain homogeneous continuous films of a given thickness. This reduces the amount of waste and the volume of solutions containing cadmium ions eliminates mixing. The equipment used is affordable and does not require the use of high temperatures and pressures, which reduces energy consumption and simplifies and reduces the cost of technology.

## EXPERIMENTAL

A mathematical model of the film's deposition process was developed based on the experiments for more efficiency and reduction of costs for its organization following existing techniques.[10-12]

Factors selected:

– $x_1$ – concentration of starting cadmium–containing salt, $c_1$, mol/L;
– $x_2$ – concentration of thiourea or sodium selenosulfate, $c_2$, mol/L;
– $x_3$ – process temperature, $T$, °C;
– $x_4$ – deposition time, $t$, min.

All chemicals used in the experiments were of high-purity grade (Se, $Cd(CH_3COO)_2$, $CdSO_4$, $CdCl_2$, $Cd(NO_3)_2$, $CdI_2$, Alfa Aesar GmbH) and of analytical grade ($NH_4OH$, $(NH_2)_2CS$, $Na_2SO_3$, Sfera Sim Ltd.) or were freshly synthesized before the experiment ($Na_2SeSO_3$).

Table III gives data on the factor levels and variation intervals. A planning matrix for full factorial experiment (FFE $3^{10}$) was compiled for the maximum detection influence of factors on the response function taking into account the effect of factors interaction. Since four factors are at 3 levels and we need to carry out 81 experiments, it is advisable to build a central compositional rotatable plan of the 2nd order (CCRP), see Table IV. The response function is the content of cadmium ions in the experimentally obtained thin films samples – *y*.

TABLE III. Factors levels and variations intervals

| The factor name | Coded designation | Factors level | | | | | Variations interval |
|---|---|---|---|---|---|---|---|
| | | –2 | –1 | 0 | +1 | +2 | |
| $c_1$ – concentration of starting cadmium-containing salt, mol/L | $x_1$ | 0.01 | 0.02 | 0.03 | 0.04 | 0.05 | 0.01 |
| $c_2$ – concentration of thiourea, mol/L | $x_2$ | 0.50 | 0.75 | 1.00 | 1.25 | 1.50 | 0.25 |
| $T$ – temperature, °C | $x_3$ | 50 | 60 | 70 | 80 | 90 | 10 |
| $t$ – time, min | $x_4$ | 1 | 2 | 3 | 4 | 5 | 1 |

TABLE IV. Central compositional rotatable plan of the 2nd order

| No. | $x_0$ | $x_1$ | $x_2$ | $x_3$ | $x_4$ | $x_1x_2$ | $x_1x_3$ | $x_1x_4$ | $x_2x_3$ | $x_2x_4$ | $x_3x_4$ | $x_1^2$ | $x_2^2$ | $x_3^2$ | $x_4^2$ | $y_1$ | $y_2$ | $y_{cp}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 1 | –1 | –1 | –1 | –1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 0.5461 | 0.5457 | 0.5459 |
| 2 | 1 | 1 | –1 | –1 | –1 | –1 | –1 | –1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1.7991 | 1.7985 | 1.7988 |
| 3 | 1 | –1 | 1 | –1 | –1 | –1 | 1 | 1 | –1 | –1 | 1 | 1 | 1 | 1 | 1 | 1.3801 | 1.3807 | 1.3804 |
| 4 | 1 | 1 | 1 | –1 | –1 | 1 | –1 | –1 | –1 | –1 | 1 | 1 | 1 | 1 | 1 | 1.8431 | 1.8436 | 1.8434 |
| 5 | 1 | –1 | –1 | 1 | –1 | 1 | –1 | 1 | –1 | 1 | –1 | 1 | 1 | 1 | 1 | 2.9211 | 2.9217 | 2.9214 |
| 6 | 1 | 1 | –1 | 1 | –1 | –1 | 1 | –1 | –1 | 1 | –1 | 1 | 1 | 1 | 1 | 4.5695 | 4.5705 | 4.5700 |
| 7 | 1 | –1 | 1 | 1 | –1 | –1 | –1 | 1 | 1 | –1 | –1 | 1 | 1 | 1 | 1 | 2.4828 | 2.4836 | 2.4832 |
| 8 | 1 | 1 | 1 | 1 | –1 | 1 | 1 | –1 | 1 | –1 | –1 | 1 | 1 | 1 | 1 | 2.8713 | 2.8723 | 2.8718 |
| 9 | 1 | –1 | –1 | –1 | 1 | 1 | 1 | –1 | 1 | –1 | –1 | 1 | 1 | 1 | 1 | 1.6245 | 1.6239 | 1.6242 |
| 10 | 1 | 1 | –1 | –1 | 1 | –1 | –1 | 1 | 1 | –1 | –1 | 1 | 1 | 1 | 1 | 5.2207 | 5.2203 | 5.2205 |
| 11 | 1 | –1 | 1 | –1 | 1 | –1 | 1 | –1 | –1 | 1 | –1 | 1 | 1 | 1 | 1 | 2.5233 | 2.5238 | 2.5236 |
| 12 | 1 | 1 | 1 | –1 | 1 | 1 | –1 | 1 | –1 | 1 | –1 | 1 | 1 | 1 | 1 | 4.5049 | 4.5059 | 4.5054 |
| 13 | 1 | –1 | –1 | 1 | 1 | 1 | –1 | –1 | –1 | –1 | 1 | 1 | 1 | 1 | 1 | 4.3119 | 4.3129 | 4.3124 |
| 14 | 1 | 1 | –1 | 1 | 1 | –1 | 1 | 1 | –1 | –1 | 1 | 1 | 1 | 1 | 1 | 4.6616 | 4.6608 | 4.6612 |
| 15 | 1 | –1 | 1 | 1 | 1 | –1 | –1 | –1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 2.6176 | 2.6184 | 2.6180 |
| 16 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 3.8286 | 3.8294 | 3.8290 |
| 17 | 1 | –2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 4 | 0 | 0 | 0 | 0.7649 | 0.7639 | 0.7644 |
| 18 | 1 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 4 | 0 | 0 | 0 | 4.8556 | 4.8548 | 4.8552 |
| 19 | 1 | 0 | –2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 4 | 0 | 0 | 3.6848 | 3.6842 | 3.6845 |
| 20 | 1 | 0 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 4 | 0 | 0 | 2.3208 | 2.3212 | 2.3210 |
| 21 | 1 | 0 | 0 | –2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 4 | 0 | 1.1612 | 1.1604 | 1.1608 |
| 22 | 1 | 0 | 0 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 4 | 0 | 2.8301 | 2.8294 | 2.8298 |
| 23 | 1 | 0 | 0 | 0 | –2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 4 | 2.9131 | 2.9125 | 2.9128 |
| 24 | 1 | 0 | 0 | 0 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 4 | 2.0433 | 2.0443 | 2.0438 |
| 25 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 2.6346 | 2.6338 | 2.6342 |
| 26 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 2.6156 | 2.6146 | 2.6151 |
| 27 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 2.6065 | 2.6061 | 2.6063 |
| 28 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 2.6518 | 2.6528 | 2.6523 |
| 29 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 2.6159 | 2.6151 | 2.6155 |
| 30 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 2.6242 | 2.6248 | 2.6245 |
| 31 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 2.6471 | 2.6475 | 2.6473 |

The experiments were randomized in time, and each experiment, according to the planning matrix of Table IV, was repeated twice.

## RESULTS AND DISCUSSION

The processing of the measurement results was carried out by the well-known methods of mathematical statistics brought to scientific research.[13–15] Each experiment was accompanied by the occurrence of errors, *i.e.*, by the reproducibility errors. Each experiment was carried out several times to assess reproducibility, so a series of parallel experiments were organized. Evaluation of the experiments' reproducibility was reduced in order to determine the dispersion of experiments' reproducibility.

Also, the randomization of experiments was carried out to eliminate systematic errors, when drawing up a plan of a matrix of the experiment. The experiments were carried out in a random sequence, which was established using a table of random numbers.

During the experiments, each of them was carried out twice, under the same conditions, in order to estimate the errors. During each experiment, the values of the averaged optimization parameters were obtained. The details are given in Supplementary material to this paper.

In order to check the adequacy and compatibility of the calculated mathematical model with the experimental results of thin film synthesis, the Fig. 2 was plotted.

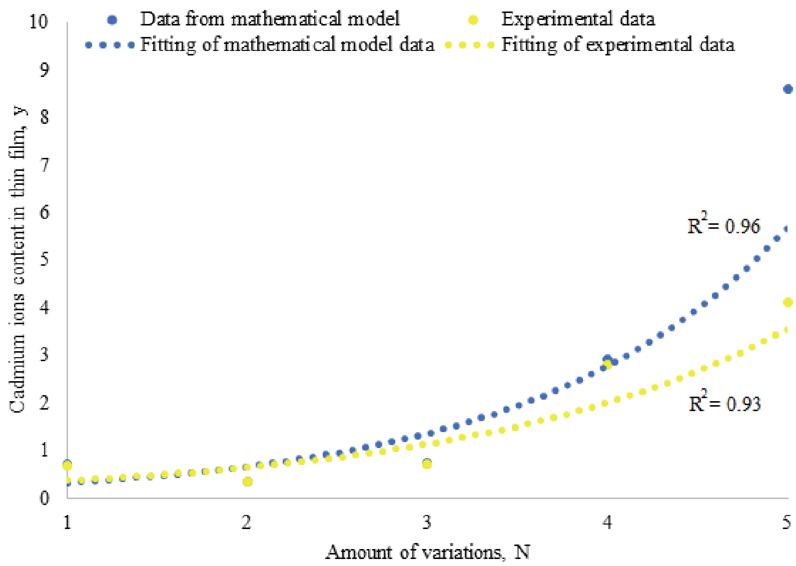


Fig. 2. Comparison of the results of mathematical modelling and experimental synthesis of thin film.

By comparing the $R^2$ factors of both dependencies, it is evident that the calculated mathematical model is appropriate, as the experimental data align closely with the values predicted by the model.

Based on the analysis of regression coefficients, it can be stated:

– a significant effect on the behaviour of the response function is exerted by the factor $x_1$ (concentration of the initial cadmium containing salt, mol/L), $x_3$ (process temperature, *T*, °C), and $x_4$ (deposition time, *t*, min), while the factor $x_2$ (concentration of thiourea, mol/L) does not have such a significant effect;

– numerical increase in the concentration of the initial cadmium containing salt; the process temperature and the deposition time lead to an increase in the response function and an increase in the concentration of thiourea - to its decrease.

As the regression equation shows, an increase in the 1$^{st}$, 3$^{rd}$ and 4$^{th}$ factor leads to an increase in the response function, and an increase in the 2$^{nd}$ factor leads to its decrease.

Based on the results of experimental studies of the content of cadmium ions (Table S-II of the Supplementary material), a nomogram is constructed.[17]

It was established that the optimum conditions, selected based on the model and confirmed according to the held experiments under which films with the highest cadmium content were produced, are:

– concentration of initial cadmium-containing salt – 0.01 mol/L;
– thiourea concentration – 1 mol/L;
– sodium selenosulfate concentration – 0.1 mol/L;
– process temperature – 70 °C;
– deposition time – 3 min.[4,5,7,18–21]

## CONCLUSION

The scientific basics for synthesizing CdS and CdSe semiconductor thin films from the aqueous solutions of cadmium-containing salts has been established through mathematical modelling of this process. An important scientific problem of great practical importance has been solved: the optimal conditions for the synthesis of CdS and CdSe thin films by the method of chemical surface deposition using the aqueous solutions of cadmium-containing salts: chloride, nitrate, sulphate, acetate and iodide have been determined. The influence of the nature of the initial salt, process temperature, deposition duration and the concentrations of salts, thiourea and sodium selenosulphate were studied. A mathematical model of chemical surface deposition of CdS and CdSe thin films as the effective photoconverters of solar radiation has been developed. The use of chemically deposited semiconductor materials of the $A^{II}B^{VI}$ type significantly reduces the cost and simplifies the process of creating solar cells, which can become the basis for the mass production of solar cells and solar battery modules. The adequacy of the obtained mathematical model was checked by Fisher's and Cochran's criteria. The optimal synthesis conditions by means of the mathematical calculations were the following: the cadmium-source salt – 0.01 mol/L; the chalcogenizer – 1.0 or 0.1 mol/L in the chase of thiourea or sodium selenosulphate, respectively; the temperature – 70 °C and the duration of 3 min.

## SUPPLEMENTARY MATERIAL

Additional data and information are available electronically at the pages of journal website: https://www.shd-pub.org.rs/index.php/JSCS/article/view/12637, or from the corresponding author on request.

## И З В О Д

## МАТЕМАТИЧКИ ПРИСТУП МЕТОДИ СИНТЕЗЕ ПОЛУПРОВОДНИЧКИХ МАТЕРИЈАЛА ФИЛМОВА ТИПА $A^{II}B^{VI}$ ЗА ФОТООСЕТЉИВЕ СТРУКТУРЕ КОЈЕ СЕ КОРИСТЕ ЗА АЛТЕРНАТИВНУ ЕНЕРГИЈУ

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Развијена је научна смерница за синтезу танких филмова CdS и CdSe методом хемијског површинског наношења (CSD), коришћењем раствора са солима које садрже кадмијум: хлорид, нитрат, сулфат, ацетат и јодид. Да би се појачала ефикасност експеримента и смањили трошкови, развијен је математички модел за CSD процес за CdS и CdSe танке филмове. Модел омогућава одређивање концентрације реагенаса, трајање и температуру CSD, који су потребни за добијање филмова одређене дебљине. Спроведена је оптимизација параметара хемијске депозиције филмастог полупроводничког материјала. На основу математичког модела, оптимални услови за синтезу су следећи: концентрација кадмијумове соли – 0,01 mol/L, халкогенизатор – 1,0 mol/L, односно 0.1 mol/L у случају тиоуреe или натријум-селеносулфата; температура – 70 °C, и трајање 3 min. Узимајући у обзир грешке, предложена је математичка зависност резултата експерименталних проучавања од садржаја металних јона у танком филму соларних ћелија за ефикасну директну конверзију сунчевог зрачења у електричну енергију.

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