Известия Гомельского государственного университета
имени Ф. Скорины, № 3 (138), 2023

Физика

УДК 539.23

Application of artificial neural networks to predict the properties of Zn_xMg_yO semiconductor sol-gel layers

Yu.V. Nikityuk[1], A.V. Semchenko[1], V.A. Prokhorenko[1], V.V. Sidsky[1], K.D. Danilchenko[1]

Using artificial neural networks the prediction of the properties of semiconductor sol-gel films of Zn_xMg_yO composition has been performed. The data arrays for working with neural networks were obtained as a result of measuring the photoelectric characteristics of sol-gel coatings on an automated basic laser test facility in accordance with GOST-17772-88. An array containing 1800 variants of input parameters was used when working with neural networks. The early stopping criterion was taken in training neural networks. The maximum number of training epochs did not exceed 1100. There are 210 neural networks with one and two hidden layers constructed during the process. The parameters of neural networks have been established that provide acceptable results in predicting the properties of semiconductor sol-gel layers. The research results can be used for determining the technological parameters of sol-gel formation processes using films with selective photosensitivity.
Keywords: neural network, sol-gel method, thin films.

С использованием искусственных нейронных сетей выполнено прогнозирование свойств полупроводниковых золь-гель пленок состава Zn_xMg_yO. Массивы данных для работы с нейронными сетями были получены в результате измерения фотоэлектрических характеристик золь-гель покрытий на автоматизированном базовом лазерном испытательном комплексе в соответствии с ГОСТ-17772-88. При работе с нейронными сетями использовался массив, содержащий 1800 вариантов входных параметров. При обучении нейронных сетей использовался критерий раннего останова. Максимальное количество эпох обучения не превысило 1100. Построено 210 нейронных сетей с одним и двумя скрытыми слоями. Установлены параметры нейронных сетей, обеспечивающие лучшие результаты при прогнозировании свойств полупроводниковых золь-гель слоев. Полученные результаты могут быть использованы при определении технологических параметров процессов формирования золь-гель методом пленок с селективной фоточувствительностью.
Ключевые слова: нейронная сеть, золь-гель метод, тонкие пленки.

Introduction. The creation of sensors, including UV sensors, is an important direction in the development of modern electronics. Such sensors find application in industry, medicine and ecology due to their ability to work under the exposure to solar radiation and radiation from heated parts of equipment. Currently intense research on materials is underway to create ultraviolet sensors, while the actual task is to develop new materials [1]–[2]. The ZnO-based thin films have photosensitivity and can be used in producing light-emitting diodes [3]–[5]. A promising option is Zn_xMg_yO films with selective photosensitivity made via the sol-gel method. The band gap width is an important characteristic of semiconductor materials. In order to change the band gap width, ZnO thin films are alloyed with various metals, including magnesium, which is suitable for replacing zinc in the lattice [6]–[7].

Presently artificial neural networks are widely used for modeling complex dependencies between input and output data of various systems. They have good capabilities to detect nonlinear relationships in multidimensional data sets [8]–[9], which makes them an effective tool for various fields of science and technology [10]–[16]. Artificial neural networks are successfully used in modeling the properties of semiconductor materials, including for predicting the properties of semiconductor sol-gel films of the Zn_xMg_yO composition when nitric acid is added to sol [16]. This paper applies artificial neural networks to predict the properties of Zn_xMg_yO semiconductor sol-gel films produced by adding hydrochloric acid to the sol.

A technique for producing sol-gel layers and measuring their photoelectric characteristics. The ZnO:Mg films were formed by separate sol-gel hydrolysis. The coatings were developed through centrifugation. Zinc acetate dihydrate, magnesium acetate, isopropyl alcohol and monoethanolamine were used as starting materials. The film-forming solution was prepared as follows: zinc acetate and magnesium acetate were dissolved separately in isopropyl alcohol and stirred at 60 °C for 10 minutes. Then, monoethanolamine was added. Similarly, magnesium acetate-based sol was produced. The sols were then mixed in different concentrations to obtain films with different component ratios (1:1, 1:2, and 1:5). As mentioned earlier, hydrochloric acid was additionally added to the sol. Silicon wafers were used as substrates during layer deposition to measure current-voltage characteristics. To determine the photocurrent, an automated basic laser test facility was used and the measurements were made in accordance with GOST-17772-88 (see figure 1). The optical module of the system included a sample positioning system, a multispectral laser radiation source made up of a set of 9 laser diodes at 405, 450, 520, 660, 780, 808, 905, 980, and 1064 nm with calibrated luminous intensity of about 2 mW. The TO-3535BC-UVC265-30-6 VE LED with a capacity of 300 µW was used as a UV source (278 nm) [17]–[18].

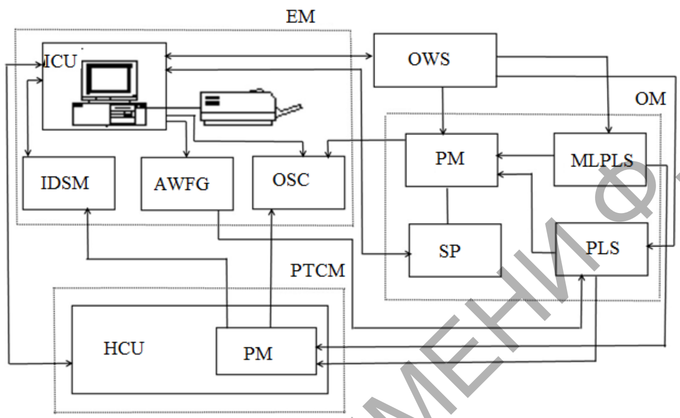

Figure 1 – Schematic diagram of an automated basic laser facility for testing photodetectors: OWS is the operator's workstation, EM is the electronics module, ICU is the information-computer unit, IDSM is the interactive digital source-meter, AWFG is the arbitrary wave-form generator, OSC is the oscillograph, OM is the optical module, PM is the positioning module, MLPLS is the multispectral laser-plasma light source, PLS is the pulsed laser source, PTCM is the positioning and thermostat control module, HCU is the heat and cold unit, PM is the positioning module, SP is the spectrophotometer

Application of artificial neural networks. The training data array and the array data for testing neural networks were formed as a result of measuring the photoelectric characteristics of sol-gel coatings in accordance with GOST-17772-88 on an automated basic laser test facility. After training, the artificial neural networks using new data sets are able to determine correctly the values of the photoelectric characteristics of the sol-gel coatings.

When working with neural networks, an array containing 1800 variants of input parameters was used, a part of which is presented in Table 1. While creating artificial neural networks, the ReLU activation function and the Adam optimizer were used to predict selective photosensitivity. The networks were formed with the MSE loss function [9]. When training the artificial neural networks, the early stopping criterion was used, with the maximum number of training epochs not exceeding 1100.

Table 1 – Section of the dataset used for training and testing artificial neural networks

№	Molar ratio		Bias voltage	Wavelength	Current strength
	Zn	Mg	U, B	λ, нм	I, A
1	1	1	-3	405	-9.260E-04
2	1	2	-6.5	450	-1.940E-03
3	1	1	-11	905	-1.140E-02
4	1	5	11	780	2.450E-05
5	1	5	-7	520	-8.150E-05
6	1	2	4	980	9.380E-05
7	1	5	-1	808	-2.120E-06
8	1	2	-1.5	405	-2.800E-04

End of Table 1

9	1	1	-5.5	450	-3.230E-03
10	1	5	-8	405	-9.380E-05
11	1	5	-11	660	-1.510E-04
12	1	2	7	780	1.220E-04
13	1	1	3.5	278	1.470E-04
14	1	5	7	520	1.030E-05
15	1	1	-0.5	660	-1.010E-05
16	1	2	-1.5	780	-3.020E-04
17	1	1	-7.5	1064	-5.710E-03
18	1	2	-14.5	660	-5,100E-03
19	1	2	-4	450	-1,080E-03
20	1	5	11	1064	2.460E-05
21	1	1	0.5	808	4.180E-06
22	1	5	-11.5	780	-1.590E-04
23	1	2	-8.5	980	-2.740E-03
24	1	1	-0.5	780	-1.020E-05
25	1	5	0.5	450	4.710E-09

During the numerical experiment, 210 neural networks with one and two hidden layers were constructed (see Figure 2).

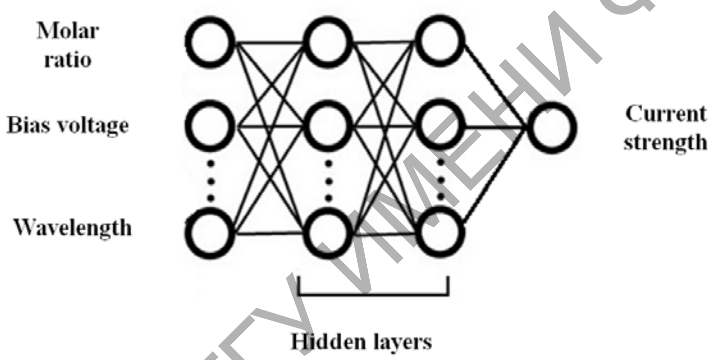

Figure 2 – Artificial Neural Network architecture

The following criteria were used to evaluate the effectiveness of artificial neural networks:

$$\mathrm{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(d_i - y_i)^2}$$ – Mean Absolute Error (MAE);

$$\mathrm{MAE} = \frac{1}{n}\sum_{i=1}^{n}\left|d_i - y_i\right|$$ – Root Mean Square Error (RMSE);

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(d_i - y_i)^2}{\sum_{i=1}^{n}(d_i - \bar{d})^2}$$ – determination coefficient.

Table 2 provides information on 20 most effective neural network configurations for predicting selective photosensitivity.

Table 2 – Artificial Neural Network Testing Results

№	Network architecture	RMSE	MAE	R^2
1	3-14-14-1	8.86E-05	5.55E-05	0.9994
2	3-14-15-1	9.05E-05	5.65E-05	0.9994
3	3-15-14-1	9.96E-05	6.23E-05	0.9993
4	3-13-15-1	1.00E-04	6.33E-05	0.9992
5	3-15-11-1	1.02E-04	6.21E-05	0.9992
6	3-15-15-1	1.02E-04	5.92E-05	0.9992
7	3-13-14-1	1.03E-04	6.30E-05	0.9992
8	3-12-14-1	1.05E-04	6.38E-05	0.9992

End of Table 2

9	3-15-12-1	1.08E-04	6.49E-05	0.9991
10	3-15-13-1	1.12E-04	6.35E-05	0.9990
11	3-13-13-1	1.15E-04	6.86E-05	0.9990
12	3-12-15-1	1.15E-04	6.21E-05	0.9990
13	3-14-13-1	1.15E-04	6.63E-05	0.9990
14	3-14-12-1	1.16E-04	7.08E-05	0.9990
15	3-15-10-1	1.16E-04	6.96E-05	0.9990
16	3-14-11-1	1.17E-04	6.43E-05	0.9990
17	3-11-13-1	1.18E-04	6.71E-05	0.9989
18	3-12-13-1	1.19E-04	7.05E-05	0.9989
19	3-13-12-1	1.20E-04	6.95E-05	0.9990
20	3-15-9-1	1.21E-04	6.91E-05	0.9989

When testing on all three selected criteria, the artificial neural network with architecture [3-14-14-1] showed the best results. Meanwhile, none of the neural networks with a configuration containing a single hidden layer was among the best networks.

Conclusion. The parameters of neural networks that provide acceptable results for predicting the properties of semiconductor sol-gel layers have been established during numerical experiments. The results obtained can be used in determining the technological parameters of sol-gel formation using the method of films with selective photosensitivity of Zn_xMg_yO.

References

1. Yuanshen, Q. Gradient bandgap narrowing in severely deformed ZnO nanopar-ticles / Q. Yuanshen [et al.] // Materials Research Letters. – 2021. – Vol. 9. – P. 58–64.

2. Liu, K. ZnO-Based ultraviolet photodetectors / K. Liu, M. Sakurai, M. Aono //Sensors. – 2010. – № 10. – P. 8604–8634.

3. Gu, K. Tailoring microstructure and optical properties of MgZnO film on glass by substrate temperature / K. Gu [et al.] // Materials Letters. – 2020. – Vol. 278. – P. 128416.

4. Priscilla, S. J. Effect of magnesium dopant on the structural, morphological and electrical properties of ZnO nanoparticles by sol-gel method / S. J. Priscilla [et al.] // Materials Today : Proceedings. – 2020. – DOI : 10.1016/j.matpr.2020.07.005.

5. A comparative analysis for effects of solvents on optical properties of Mg doped ZnO thin films for optoelectronic applications / F. Baig, M. W. Ashraf, A. Asif, M. Imran // Optik. – 2020. – Vol. 208. – P. 164534.

6. Loeza-Poot, M. Novel sputtering method to obtain wide band gap and low resistivity in as-deposited magnesium doped zinc oxide films / M. Loeza-Poot [et al.] // Materials Science in Semiconductor Processing. – 2019. – Vol. 104. – P. 104646. – DOI :10.1016/j.mssp.2019.104646.

7. Asvarov, A. Sh. Structural and optical properties of Mg doped ZnO thin films deposited by DC Magnetron Sputtering / A. Sh. Asvarov [et al.] // Journal of Nano- and Electronic Physics. – 2016. – Vol. 8. – P. 04053.

8. Golovko, V. A. Neural network technologies for data processing : textbook. allowance / V. A. Golovko, V. V. Krasnoproshin. – Minsk : BSU, 2017. – 263 p.

9. Chollet, F. Deep Learning with Python / F. Chollet. – USA : Manning Publications Co., 2018. – P. 400.

10. Bakhtiyari, A. N. A review on applications of artificial intelligence in modeling and optimization of laser beam machining / A. N. Bakhtiyari, Z. Wang, L. Wang, H. Zheng // Optics & Laser Technology. – 2021. – Vol. 135. – P. 1–18.

11. Application of artificial neural networks and finite element method for determining the parameters of elliptic laser beam treatment of quartz sol-gel glasses / Y. V. Nikitjuk, A. N. Serdyukov, V. A. Prohorenko, I. Y. Aushev // Problems of Physics, Mathematics and Technology. – 2021. – № 3 (48). – P. 30–36. – DOI : 10.54341/20778708_2021_3_48_30.

12. Application of finite element method and artificial neural networks to determine laser treatment parameters for 12X18H9T Steel / Yu. V. Nikitjuk, G. A. Baevich, V. N. Myshkovets [et el.] // Vestnik of the Sukhoi State Technical University of Gomel. – 2022. – № 1 (88). – P. 48–55.

13. Nikitjuk, Yu. V. Determination of the parameters of two-beam laser splitting of silicate glasses using regression and neural network models / Yu. V. Nikitjuk, A. N. Serdyukov, I. Y. Aushev // Journal of the Belarusian State University. Physics. – 2022. – № 1. – P. 35–43. – DOI : 10.33581/2520-2243-2022-1-35-43.

14. Determination of the parameters of dual-beam laser cleaning of quartz raw materials using artificial neural networks and the finite element method / Yu. V. Nikitjuk, E. B. Shershnev, S. I. Sokolov, I. Y. Aushev // Problems of Physics, Mathematics and Technics. – 2022. – № 3 (52). – P. 37–41.

15. Characterization of laser welding of steel 30ХГСН2А by combining artificial neural networks and finite element method / Y. Nikitjuk, G. Bayevich, V. Myshkovets [et al.] // Lecture Notes in Networks and Systems. – 2022. – Vol. 422. – P. 273–279. – DOI : 10.1007/978-981-19-0379-3_28.

16. Predicting the properties of Zn_xMg_yO semiconductor sol-gel layers using artificial neural networks / Yu. V. Nikitjuk, A. V. Semchenko, V. V. Sidsky [et el.] // Problems of Physics, Mathematics and Technics. – 2022. – № 1 (50). – P. 28–32. – DOI : 10.54341/20778708_2022_1_50_28.

17. Photoactive properties of ZnOx : MgO nanocomposite coatings deposited in vacuum and by sol-gel method / V. V. Malyutina-Bronskayaa, A. V. Semchenkob, A. V. Rogachev, M. A. Yarmolenko, V. V. Sidskiy, K. D. Danilchenko, S. A. Sorokaa, E. V. Rusu // PFMT. – 2021. – Is. 2 (47). – P. 39–44.

18. Malyutina-Bronskayaa, V. V. Automated basic laser test facility for testing advanced types of semiconductor photodetectors / V. V. Malyutina-Bronskayaa [et el.] // Proceedings of the 13th International Scientific and Technical Conference «Instrumentation –2020», Minsk, November 18–20 2020. – Minsk : BNTU. – 2020. – P. 391–392.

Гомельский государственный
университет имени Франциска Скорины

Поступила в редакцию 24.10.2022