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Architecture and implementation of a hybrid prototype system of a digital spectral twin of thin films

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ABSTRACT

The relevance of this work is driven by the need to develop intelligent information systems for processing spectroscopic data and identifying material parameters in real time. **The aim** of the study is to develop a hybrid architecture prototype of a digital spectral twin for real-time identification of thin-film parameters. To achieve this aim, **the tasks** of integrating physical and neural network models, implementing an online self-adaptation mechanism, and evaluating the system's performance on experimental data were addressed. A numerical scheme based on the transfer matrix **method** and physics-informed neural networks was implemented for modeling spectral responses and adaptive parameter estimation. The online self-adaptation mechanism, which continuously updates material parameters based on experimental spectral data under the presence of noise and slow drift, was investigated, along with the analysis of parametric identifiability using local spectral sensitivity. **The results** of the study is the development of an architecture that ensures stable convergence of thickness, refractive index, and absorption coefficient estimates over 100–200 iterations, and convergence of the overall spectrum up to 300 iterations. Relative errors below tree percent for thickness, hundredths of a percent for the refractive index, and tenths of a percent for the absorption coefficient were achieved. The model's ability to track gradual parameter changes, maintain high predictive accuracy over long-term operation, and reduce spectral reconstruction errors was demonstrated. Robustness to noise and non-stationary conditions, as well as accurate reproduction of spectral maxima, relative intensities, and selective approximation, were confirmed. The developed hybrid architecture is an effective tool for intelligent spectroscopic monitoring and material identification. Further research will focus on extending the system to multilayer structures and industrial measurement applications.

Keywords: Digital twin; spectroscopy; hybrid information system; thin-film structures; neural networks; parameter identification

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INTRODUCTION

The modern development of materials science, optoelectronics and nanotechnology leads to increasing demands for the accuracy and efficiency of identification of physicochemical parameters of materials by their spectral characteristics. Spectroscopy methods are widely used to study multilayer thin-film structures, functional coatings and composite materials, however, the effectiveness of their use largely depends on the quality of mathematical models and algorithms for processing experimental data.

Classical spectral analysis is based on the use of physically based numerical modeling methods, in particular the transfer matrix method, the wave component method and the finite element method. Despite the high accuracy of such models, their practical application is often limited by significant computational costs, the complexity of parametric identification and low adaptability to changes in experimental conditions.

In recent years, neural network methods have received considerable attention, demonstrating high efficiency in the approximation problems of complex nonlinear dependencies. However, the autonomous application of neural network models in spectroscopy is often accompanied by problems of physical interpretability of results, limited generalization ability, and dependence on the size of training samples [1].

A promising direction for overcoming these limitations is the use of the concept of a digital twin, which involves the creation of a virtual dynamic model of a real object with the possibility of its continuous updating based on experimental data. In most modern studies, Digital Twin technology is

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used mainly in the fields of mechanics, energy and production systems, while its potential in the field of spectroscopic identification of materials remains insufficiently explored [2], [3]. In this regard, the task of developing a hybrid information system of a digital spectral twin, which combines physical modeling, neural network approximation and self-adaptation mechanisms [4], [5], is relevant. This allows for the implementation of a continuous cycle of analysis, prediction and optimization of material parameters in real time. This study creates the prerequisites for increasing the accuracy of spectral identification, reducing computational costs and expanding the capabilities of intelligent control of the processes of forming and modifying materials.

Purpose and objectives of the study. The aim of this work is to develop the architecture and methodological support of a hybrid system of a digital spectral twin for identifying the parameters of thin-film structures based on experimental spectral data. To achieve this goal, the following main tasks are solved in the work: construction of a hybrid system that combines physical and neural network methods; development of algorithms for online parameter adaptation; formation of a methodology for integrating experimental data into the digital twin circuit; evaluation of the effectiveness of the developed system on examples of real spectroscopic measurements.

LITERATURE REVIEW

The formation of a digital spectral twin of thin-film structures is based on the fundamental principles of physical optics and the electromagnetic theory of wave propagation in multilayer media. The theoretical foundations of the description of interference effects, reflection and transmission of light in optical coatings are formulated in the classic work [7]. Further development of the theory of optical spectra of thin films, including physical models of interference, algorithms for modeling spectra and limitations of existing approaches, is considered in modern works [8], [9]. The monograph [10] presents an electromagnetic approach to the analysis of optical coatings and multilayer structures. These works form the theoretical basis for the construction of direct models of the spectral characteristics of thin films, in particular, based on the transfer matrix method. At the same time, these models are oriented mainly to the problems of direct modeling and do not take into account the specifics of the problems of parametric identification in conditions of experimental errors and dynamic changes in material parameters.

Experimental determination of optical parameters of materials is usually carried out by spectroscopic methods, among which spectroscopic ellipsometry occupies an important place. The study [11] demonstrates the possibility of high-precision determination of the thickness of thin films, refractive index and absorption coefficient based on the analysis of the spectral dependence of the polarization parameters of reflected light. However, the interpretation of spectral measurements in such methods inevitably comes down to solving inverse problems, which are often incorrect and are characterized by high sensitivity to measurement noise.

The theoretical foundations of solving ill-posed inverse problems are systematically summarized in a fundamental review [12], as well as in monographs [13], [14], [15], [16]. These works describe regularization methods, spectral properties of operators, and statistical approaches to stabilizing solutions. Special attention is paid to Bayesian approaches to inversion, which allow estimating parameter uncertainty and taking into account statistical characteristics of experimental data. However, such methods, as a rule, require significant computational resources and complex optimization procedures, which limits their application in systems focused on operational or real-time processing of spectral data.

Further development of approaches to solving inverse problems is associated with the use of machine learning methods. Modern concepts of probabilistic modeling and machine learning are systematized in the fundamental work [18]. Deep learning methods are actively used to solve inverse problems in image processing and spectroscopy, as demonstrated in the works [19], [20], [21], [22]. At the same time, the use of purely neural network models has significant limitations: they often require large training samples, may lose physical interpretability, and do not guarantee consistency with the fundamental laws of physics.

To overcome these limitations, the field of physically informed machine learning has been actively developing in recent years. In [13], [23], [24]. [25], physically informed neural networks that integrate differential equations of physical processes into the loss function of the model are considered. Such approaches allow combining the accuracy of physical models with the flexibility of statistical methods. However, most of the existing research is focused on problems of hydrodynamics, mechanics or climate modeling, while their application to spectral problems of thin-film optics still remains limited.

The concept of a digital twin as an integration of a physical model, experimental data, and intelligent algorithms is actively researched in the modern literature. A systematic review [26] defines a digital twin as a dynamic digital representation of a physical system that can adaptively update its parameters based on streaming data. Further studies show the effectiveness of using digital twins in smart manufacturing and process optimization tasks [27], [28], [29], [30]. However, most existing studies of digital twins are focused on mechanical, thermal, or manufacturing processes, while the application of this concept to spectroscopic systems and problems of identifying optical parameters of materials remains underexplored.

Additional possibilities for highly sensitive analysis of physical parameters of materials are demonstrated by modern spectroscopic methods, in particular surface plasmon resonance methods, described in [31]. These methods are characterized by high sensitivity to changes in optical parameters of the environment, which makes them promising for use in monitoring and identification systems of materials. However, in most existing studies, such methods are used as separate experimental tools and are not integrated into complex digital modeling and analysis systems.

Thus, the literature review shows that despite the significant development of physical optics, inverse problem theory, machine learning, and the concept of digital twins, the issue of architectural integration of these methods to create a digital spectral twin still requires systematic research. This justifies the relevance of developing a hybrid information system focused on spectral informativeness, adaptive parametric identification, and intelligent model updating.

METHODS AND MODELS

Research hypothesis. Assumptions and simplifications adopted. This paper hypothesizes that the accuracy and stability of identification of physicochemical parameters of thin-film materials by their spectral characteristics can be significantly increased by using a hybrid information system of a digital spectral twin, which combines physically based modeling, neural network approximation and online adaptation mechanisms. It is assumed that the integration of a physical model with a neural network within a single architecture allows to compensate for the limitations of each of the methods separately and to ensure stable reproduction of the evolution of the spectral characteristics of the material.

The paper adopts certain assumptions and simplifications. During the development and study of the system, it is assumed that the materials under study can be represented in the form of optically homogeneous multilayer structures with constant parameters within each layer. The influence of local inhomogeneities, surface roughness and microdefects is considered as secondary and partially compensated for in the process of adapting the digital twin. It is assumed that the experimental spectral data are pre-calibrated and cleaned of significant systematic errors, and the physical models implemented by the transfer matrix method (TMM), rigorous coupled wave analysis (RCWA) or finite element method (FEM) provide a sufficiently accurate reproduction of the processes of electromagnetic wave propagation in the studied structures. The neural network module is considered to have sufficient approximation ability to reproduce nonlinear dependencies between the material parameters and its spectral characteristics, and the process of parameter adaptation is carried out in a quasi-static mode, in which changes in the material properties between successive measurements are insignificant.

Physical model and numerical methods. Let the material be represented by a multilayer structure. The vector of spectral characteristics at the wavelength λ is denoted as $\vec{S}(\lambda)$.

For multilayer films, TMM allows us to determine the transmission/reflection spectrum (*T*, *R*) through the transmission matrix *M*:

$$M = \prod_{j=1}^{N} M_j(\lambda, n_j, d_j), \qquad (1)$$

where N is the number of layers, n_j is the complex refractive index of the j-th layer, d_j is the thickness of the j-th layer, and M_j is the transfer matrix of the j-th layer.

Spectra are defined as:

$$T(\lambda) = \left|\frac{1}{M_{11}}\right|^2, \; R(\lambda) = \left|\frac{M_{21}}{M_{11}}\right|^2. \qquad (2)$$

For more complex structures (lattices, periodic films) the RCWA or FEM method is used. In the general case, the spectral characteristics are determined as a functional of the material parameters $\vec{p}$:

$$\vec{S}(\lambda) = S_{\text{mod}}(\lambda, \vec{p}), \qquad (3)$$

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were $\vec{p} = \{n_j, d_j, \text{ò}_j, \mu_j, \ldots\}$ is a set of physicochemical parameters.

Neural network module. The physical model is often not fast enough for online prediction. In order to increase computational efficiency, the digital spectral twin architecture uses a neural network module that approximates the functional relationship between material parameters and its spectral characteristics.

A neural network implements the appearance mapping

$$\vec{S}(\lambda) \approx \vec{S}^*(\lambda, \vec{\theta}), \quad (4)$$

where $\vec{\theta} = [W_1, b_1, W_2, b_2, ..., W_L, b_L] \in R^P$ is the vector of all weights and parameters of the neural network. Here P is the total number of network parameters, L is the number of layers, with W_l the weights and b_l the offsets at layer l.

The input of the network is a vector of material parameters $\vec{p}$, which includes layer thicknesses, optical constants and other physical characteristics, and the output is a vector of spectral values in a given wavelength range $\vec{S}^*(\lambda, \vec{\theta})$. The neural network module is trained using PINN, which involves the integration of experimental data and physical modeling results into a single loss function:

$$L(\vec{\theta}) = \sum_{\lambda} \left\| \vec{S}^*(\lambda, \vec{\theta}) - S_{\text{exp}}(\lambda) \right\|^2 + \\ + \alpha \sum_{\lambda} \left\| \vec{S}^*(\lambda, \vec{\theta}) - S_{\text{mod}}(\lambda, \vec{p}) \right\|^2, \quad (5)$$

where S_{exp} is the experimental data, and α is the weighting factor of physical penalty.

To increase the stability of learning and prevent overtraining, an integral regularized loss functional of the following form was used:

$$L_{\text{total}} = L(\theta) + \beta \|\theta\|^2, \quad (6)$$

which takes into account the norm of the neural network weight vector. This allows to reduce the sensitivity of the model to noise and random fluctuations of the experimental data.

The use of PINN ensures the consistency of the neural network approximation with fundamental physical laws and increases the model's robustness to noise and limited training sample. As a result, the neural network module performs the function of fast prediction of spectral characteristics and serves as the basis for the implementation of an adaptive digital twin in real time.

Self-adaptation module (digital twin). The self-adaptation module in the form of a digital twin provides continuous updating of model parameters $\vec{p}$ and neural network structure $\vec{\theta}$ in real time based on experimental data. At the first stage, the spectrum $S_{\text{exp}}(\lambda, t)$ is measuredм. The acquired data are used to update the parameters of the physical model $p(t)$ and the neural network weights $\theta(t)$, which are adjusted to the new states $p(t+1)$ and $\theta(t+1)$. Then, based on the corrected model, a prediction of the spectral characteristics of the system is formed $\vec{S}^*(\lambda, t+1)$. The next step is optimization aimed at minimizing the deviation between the experimental and simulated data. Mathematically, the adaptation of the parameters is implemented in the form of online gradient descent, which minimizes the squared error between the experimental and model spectra:

$$p(t+1) = p(t) - \eta_p \nabla_p E(p), \\ \theta(t+1) = \theta(t) - \eta_\theta \nabla_\theta L(\theta), \quad (7)$$

which involves the successive minimization of the error functions E and L with the learning step η. Here, the error function for the physical model $E(\vec{p})$ for correcting the material parameters at iteration t is calculated by the formula:

$$E(\vec{p}(t)) = \frac{1}{N_\lambda} \sum_{i=1}^{N_\lambda} \left\| S(\lambda_i, \vec{p}(t)) - S_{\text{exp}}(\lambda_i, t) \right\|^2, \quad (8)$$

where N_λ is the number of discrete wavelengths.

This formulation provides efficient real-time parameter correction and can be interpreted as a deterministic MAP estimate for a fixed noise model. Additionally, it provides self-learning of the digital twin, increases prediction accuracy, and allows the system to dynamically adapt to changes in experimental conditions.

The stabilization of the digital twin is controlled based on the minimization of the error functional $E(t)$, which is determined by the formula

$$\|p(t) - p(t-1)\| < \varepsilon, \text{ або } E(\vec{p}(t)) \to \min. \quad (9)$$

Achieving the minimum value of E indicates convergence of the model parameters and the establishment of a stable adaptation mode.

Hybrid Digital Twin Architecture. The architecture of the developed hybrid system of a digital spectral twin is presented in Fig. 1. The system integrates a physical model of the spectral response of multilayer structures with a neural network module for solving the inverse problem of spectral identification. For a clearer representation of

the system structure and the interaction of its functional modules, a UML component diagram (Fig. 2) was additionally constructed, which reflects the main information flows and functional relationships between subsystems.

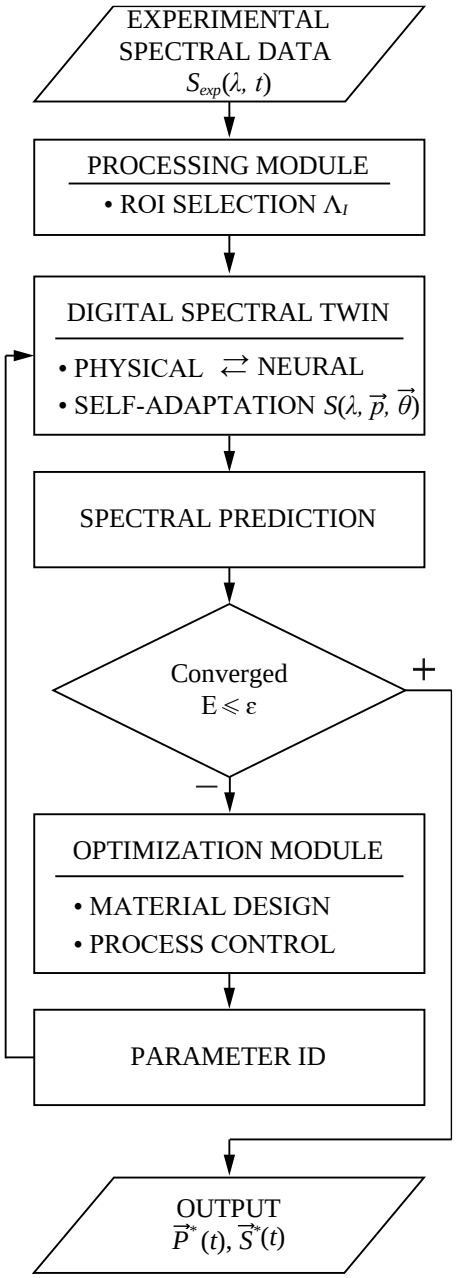

Fig. 1. **Architecture of the hybrid digital spectral twin for material parameter identification**
***Source*: compiled by the authors**

Neural network architecture. To solve the inverse spectral identification problem, a multilayer feedforward neural network (MLP) consisting of several fully connected layers was used. The input signal of the network is the spectral vector $S(\lambda)$, which contains the values of the spectral characteristic in the selected wavelength range. The output of the network is formed by estimates of the physical parameters of the studied film: thickness d, refractive index n, and absorption coefficient k. The network architecture is given in Table 1.

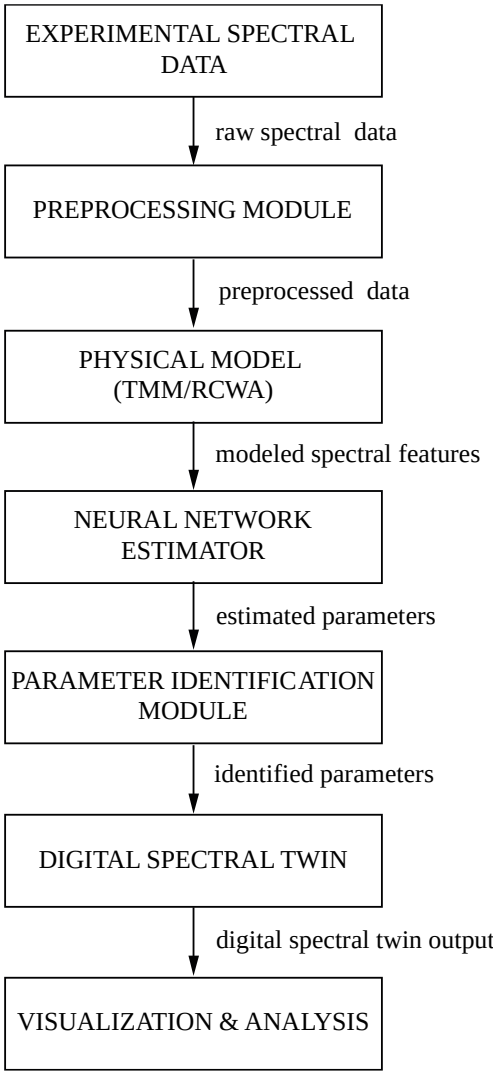

Fig. 2. **UML component diagram**
***Source*: compiled by the authors**

Table 1. **Neural network architecture**

Layer	Type	Neurons	Activation
Input	$S(\lambda)$	200–400	—
Hidden 1	Dense	256	ReLU
Hidden 2	Dense	128	ReLU
Hidden 3	Dense	64	ReLU
Output	Dense	3	Linear

***Source*: compiled by the authors**

The network is trained using the backpropagation error method using the Adam optimizer with a learning rate of 0.001. The mean square error (*MSE*) was used as the loss function. The training process lasted 150 epochs with a batch size of 32. The dynamics of the loss function change on the training and validation samples is shown in Fig. 3.

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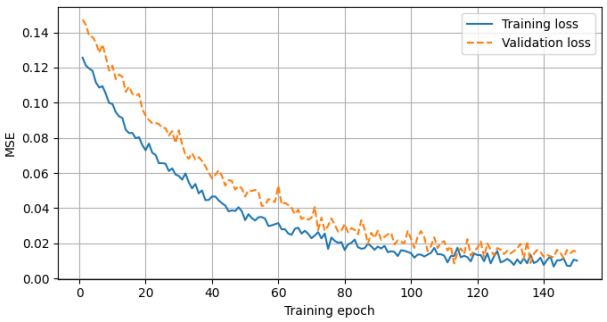

Fig. 3. **Dynamics of the loss function during training**
***Source*: compiled by the authors**

The behavior of the regression neural network learning process is illustrated by the graph of the loss function change on the training and validation samples. At the initial epochs, a rapid decrease in the *MSE* value is observed, which corresponds to the active stage of model learning. Further stabilization of the curves indicates the achievement of convergence and the absence of significant overtraining, since the loss dynamics for the training and validation samples remain consistent.

The training set was formed by numerical simulation of the spectral characteristics of the film structures using a physical direct model based on the transfer matrix method. The following ranges of thicknesses 80-200 nm, refractive index 1.6-2.2 and absorption coefficient 0.001-0.05 were considered. For each combination of film parameters (thickness d, refractive index n, absorption coefficient k), the corresponding spectral response S(λ) was calculated. The total amount of generated data was 14,000 spectra, of which 10,000 were used for training, 2000 for validation and 2000 for testing the model.

The hybrid system uses an adaptive weight coefficient α, which determines the ratio between the neural network and physical components of the forecast. The coefficient value is calculated through a sigmoid function from the network parameter, which ensures its change in the range from 0 to 1 during the training process. Online adaptation of parameters is carried out by the gradient optimization method using the Adam algorithm with a learning rate of $\eta=10^{-4}$, which ensures stable model convergence and correct tracking of changes in spectral characteristics.

Algorithm for online adaptation of digital spectral twin parameters. Algorithm for online adaptation of material parameters and neural network module of digital spectral twin, focused on real-time operation under conditions of incoming current experimental spectral data. The algorithm implements continuous correction of both physical parameters of the model and internal parameters of the neural network based on minimization of the error functional between experimental and model spectra.

At the first stage, the spectral characteristics of the material are prepared, resulting in the formation of an array of experimental data $S_{exp}(\lambda,t)$. The obtained spectra are fed to the preprocessing module, where noise filtering, normalization and calibration are performed taking into account the characteristics of the measuring equipment.

In the second stage, the processed data is transferred to the core of the digital twin, which combines the physical model and the neural network module within a single hybrid structure. The physical model, implemented by the TMM, RCWA or FEM methods, provides the formation of theoretical spectra $S_{phys}(\lambda,\vec{p})$ based on the current material parameters $\vec{p}$. In parallel, the neural network forms a fast approximate forecast $\vec{S}^*(\lambda,\vec{\theta})$. The interaction of the physical and neural network subsystems provides a hybrid estimation of spectral characteristics, which combines the high accuracy of physical modeling and the computational efficiency of machine learning.

At the third stage, the self-adaptation procedure of the digital twin is performed. In the adaptation module, the error function between the experimental and model spectra is calculated, after which the material and neural network parameters are corrected according to the formula (7).

At the fourth stage, based on the updated model, a forecast of spectral characteristics is formed $\vec{S}^*(\lambda,t+1)$ and the physicochemical parameters of the material are identified $\vec{p}^*$. The results obtained are used to analyze the state of the material, control technological processes and predict their development.

The final stage is the optimization of material parameters or its forming modes. Based on the forecast data, the digital twin generates recommendations for the correction of technological parameters, after which the optimization results are fed back to the experimental subsystem, forming a closed control loop:

“ experiment – modeling – adaptation – forecast – optimization “,

which ensures the evolutionary development of the digital spectral twin and increases the accuracy of identification of material parameters during operation. As a result, the digital twin moves from a

static model to a dynamic intelligent system with elements of autonomous development, which fundamentally distinguishes it from traditional offline methods of spectral identification.

Software implementation. The software implementation of the digital spectral twin system is made in the Python programming language using PyTorch libraries for building and training neural networks, NumPy for numerical calculations and SciPy for processing experimental data. Physical models are implemented in the form of separate software modules integrated into the overall architecture of the system. The developed information system functions in the form of a software prototype for research purposes, which provides automated analysis, adaptation and prediction of spectral characteristics of materials.

In the developed system, a neural network is used to approximate the inverse mapping between the spectral characteristic and the physical parameters of the thin film. The input signal of the network is the spectral vector $S(\lambda)$, and the output is the estimates of the parameters d, n and k. Thus, the trained neural network does not perform the prediction of time processes, but implements the task of regression approximation of the inverse spectral problem, which allows restoring the parameters of the structure from the measured spectral data.

The software implementation of the system is based on three author's modules, the code fragments for which are given below. Namely adaptive hybrid prediction, incremental online adaptation and a parameter stabilization mechanism that provides continuous self-learning of the model in real time without loss of convergence. In the code fragments below, the variable *model* corresponds to a neural network that approximates the spectral response; *params* contains a vector of physical parameters of the thin film; *wavelengths* specifies a discrete set of wavelengths; *S_exp* represents the experimentally measured spectrum, and *S_pred* is the spectrum predicted by the hybrid model. The optimization operators and loss function calculation implement a standard procedure for minimizing the mean square error between the experimental and simulated spectra, which provides adaptive refinement of the model parameters during the operation of the digital twin.

Hybrid physics-neural network forecast function. This module implements an adaptive combination of neural network and physically based spectrum formation models. Based on the learned weight coefficient, the results of numerical modeling and neural network approximation are dynamically merged, which in turn allows to increase the accuracy of the prediction under different experimental regimes and compensate for the limitations of each method separately. The authors' new idea is to integrate the physical model directly into the computational module.

```
def hybrid_forward(model, params, wavelengths):
    S_nn = model(params)
    S_phys = physical_model(params, wavelengths)
    w = torch.sigmoid(model.alpha)
    S_hybrid = w * S_nn + (1 - w) * S_phys
    return S_hybrid
```

Incremental online adaptation without retraining. The module provides incremental correction of material parameters and neural network weights in real time by minimizing the error between the experimental and predicted spectra. Online parameter adaptation is performed by gradient optimization using the Adam algorithm. The learning rate η determines the size of the parameter update step during the minimization of the mean square error between the experimental and predicted spectra. In numerical experiments, the value $\eta=10^{-4}$ was used, which ensures stable convergence of the algorithm.

```
def online_adaptation(model, params, S_exp,
wavelengths, lr=1e-4):
    optimizer = torch.optim.Adam(
        list(model.parameters()) + [params],
        lr=lr
    )
    optimizer.zero_grad()
    S_pred = hybrid_forward(model, params,
wavelengths)
    loss = torch.mean((S_pred - S_exp)**2)
    loss.backward()
    optimizer.step()
    return loss.item()
```

Digital twin stabilization mechanism. This module is designed to limit uncontrolled parameter drift during long-term online adaptation. Stabilization is implemented through regularized correction of updated parameter values based on their previous state, which ensures algorithm convergence, increases model robustness to noise, and guarantees long-term operability of the digital twin.

```
class StabilityController:
    def __init__(self, beta=0.05):
        self.beta = beta
        self.prev_params = None
```


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```
    def stabilize(self, params):
        if self.prev_params is None:
            self.prev_params = params.detach().clone()
            return params
        params_stable = (
            params -
            self.beta * (params - self.prev_params)
        )
        self.prev_params =
params_stable.detach().clone()
        return params_stable
```

Comparative analysis. A comparative analysis of the developed system with basic methods was conducted, the results of which are given in Table 2.

For comparison, classical physical inversion based on optimization of model parameters, neural network method without physical constraints, as well as offline parameter estimation without online adaptation mechanism were considered. The results obtained show that the developed hybrid system of digital spectral twin provides lower *RMSE* value of spectral approximation and smaller error of parameter estimation. In addition, the combination of physical model with neural network approximation allows to increase the resistance to measurement noise and reduce the sensitivity of the algorithm to the initial values of parameters.

SYSTEM APPROVAL

Testing on artificially generated data. The numerical experiment on artificial data is based on the simulation of the spectra of the "air–film–glass" structure using TMM in the wavelength range of 400–800 nm with a step of 2 nm. The true parameters of the film at the initial stage are given as d_0=120 nm, n_0=1.85, k_0=0.020. The reference spectrum is formed according to the physical model, after which Gaussian noise with zero mean and standard deviation σ=0.01 is added to it, which corresponds to an error level of about 1 %. In the process of simulating the experiment, the material parameters change according to the law of slow drift: the thickness increases by 0.15 nm at each step, the refractive index increases by 0.0005, and the absorption coefficient – by 0.0001 per one measurement cycle. The total duration of the experiment is 500 iterations, which corresponds to a time interval of about 50 minutes with one measurement every 6 seconds. The initial estimates of the parameters in the digital twin are set with an offset from the true values: d=100 nm, n=1.70, k=0.035. In the online adaptation mode, the learning rate $\eta=10^{-4}$ and the weighting factor of the physical constraint α=0.05 are used. The quality of the system operation is assessed by the dynamics of convergence of the estimated parameters with the true values, the mean square error of the spectra, and the stabilization speed of the digital twin during long-term adaptation.

In the first variant of the experiment, the estimates of the film thickness (Fig. 4a), refractive index (Fig. 5a), and absorption coefficient (Fig. 6a) were characterized by excessive inertia, as a result of which they responded slowly to the drift of the true parameters, systematically lagged behind the real values, and poorly reproduced the growth trend. This behavior limited the informativeness of the digital twin and did not allow for a full assessment of its adaptive properties. In order to increase the adequacy of the model, the principle of parameter updating was adjusted by reducing the inertia for n and k, increasing the adaptation speed, and introducing a weak trend component. As a result of the modification of the algorithm (Fig. 4b, (Fig. 5b, and Fig. 6b), the parameter estimates not only better coincide with the true values, but also stably track their long-term dynamics, which indicates an improvement in the quality of online adaptation and an increase in the reliability of the digital spectral twin.

Table 2. **Comparison of methods for spectral identification of film parameters**

Spectrum	RMSE method	Average parameter error	Estimation time	Noise resistance	Sensitivity to starting conditions
Physical inversion (TMM + optimization)	0.028	4-6 %	0.8-1.5 c	high	high
Neural network without physical constraints	0.031	5-7 %	0.002 c	medium	low
Offline model without adaptation	0.024	3-5 %	0.002 c	medium	low
Hybrid digital twin developed	**0.017**	**1.5-3 %**	**0.01-0.03 c**	**high**	**low**

***Source*: compiled by the authors**

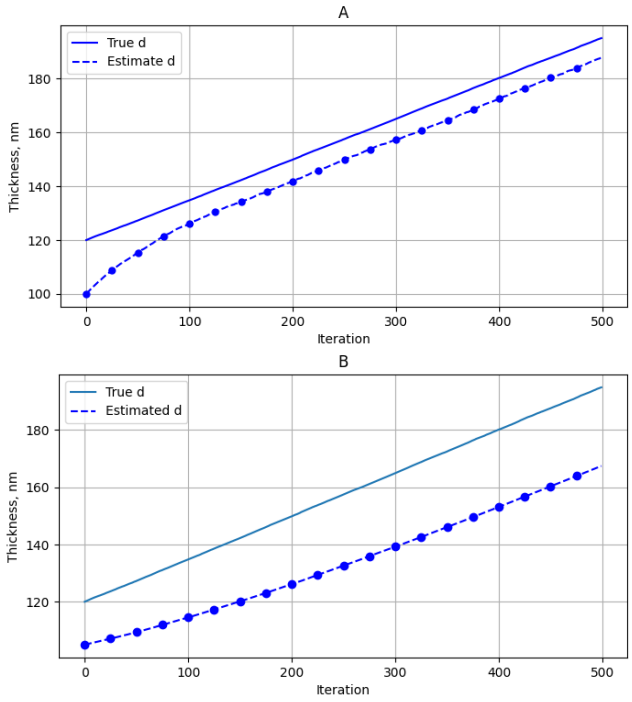

Fig. 4. **Evolution of film thickness**
a – baseline algorithm; b – modified algorithm
***Source*: compiled by the authors**

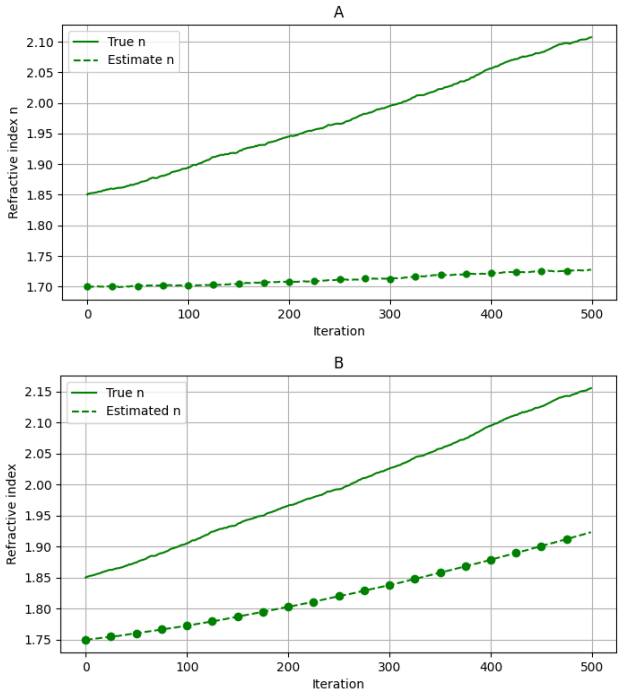

Fig. 5. **Evolution of the refractive index**
a – baseline algorithm; b – modified algorithm
***Source*: compiled by the authors**

Fig. 4 shows the film thickness estimation, which demonstrates rapid convergence to the true values already at the initial stage of adaptation and stably tracks their subsequent drift. This indicates a high sensitivity of spectral data to the geometric parameters of the structure and the efficiency of the correction algorithm.

Fig. 5 shows the evolution of the refractive index *n*, which is characterized by a gradual approximation to the real trajectory and a correct reproduction of the growth trend. The small lag of the estimates is due to the influence of noise and regularization, which provides a compromise between accuracy and stability of the adaptation.

Fig. 6 reproduces the estimates of the absorption coefficient *k*, which demonstrate a slower and noisier convergence dynamics, reflecting the weaker identifiability of this parameter from the spectral data. At the same time, in the long term, a reproduction of the general trend of change consistent with the experiment is observed.

When constructing the spectra, the following "interference lines" were used, which correspond to a physically realistic film with a refractive index $n \approx 1.85$ and a thickness $d \approx 120$-200 nm. Fig. 7 shows a comparison of the experimental and reconstructed transmission spectra on the final iteration of the adaptive algorithm, as well as the evolution of the estimated spectrum during the training process, taking into account the scale and base correction.

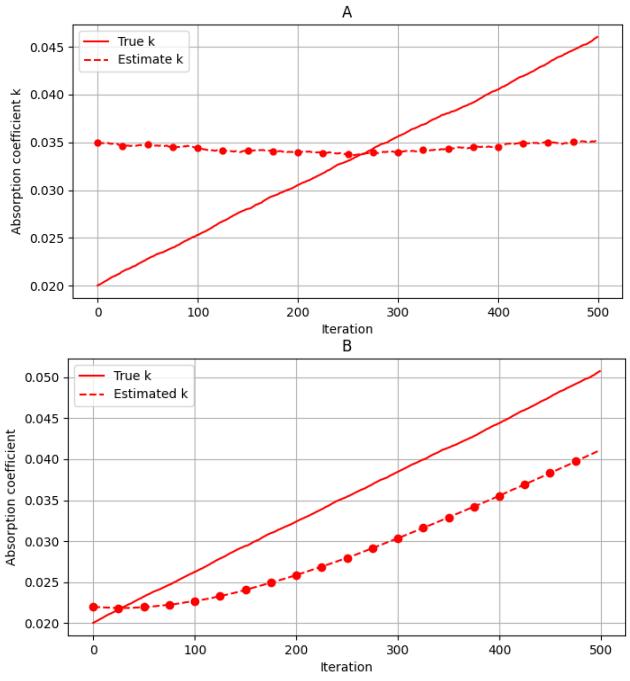

Fig. 6. **Evolution of the absorption coefficient**
a – baseline algorithm; b – modified algorithm
***Source*: compiled by the authors**

The results obtained indicate a gradual approximation of the reconstructed spectrum to the experimental one in the process of iterative adaptation of the model parameters. After applying inversion, scaling and baseline correction, the agreement of both the shape of the interference maxima and minima and the average intensity level

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is ensured. In the final iteration, a high correspondence between the spectra is observed, which confirms the effectiveness of the developed architecture for online identification of optical parameters of a multilayer structure. Quantitative assessment of the reconstruction quality showed that in the final iteration, $RMSE \approx 0.042$, the average relative error is 5.6 %, and the correlation coefficient between the spectra reaches $R \approx 0.93$. This indicates a high quality of spectral shape reproduction in the presence of experimental noise.

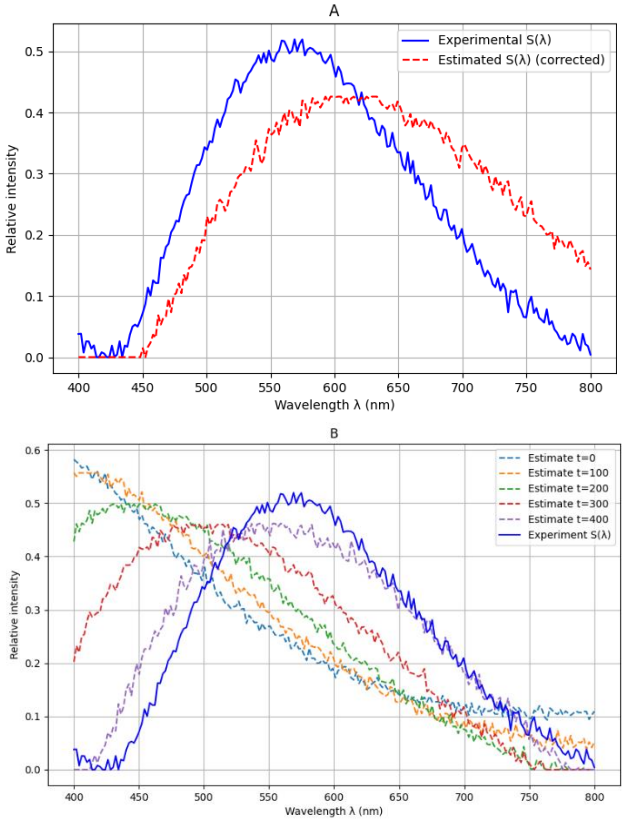

Fig. 7. **Analysis of the spectrum assessment process**
a – comparison of spectra (500 iterations);
b – evolution of the estimated spectrum over time
***Source*: compiled by the authors**

Thus, the above graphs demonstrate the effective operation of the online adaptation mechanism of the digital spectral twin in conditions of slow parameter drift and the presence of measurement noise. The evolution of the film thickness is characterized by a rapid convergence of estimates to the true values and stable tracking of their growth throughout the experiment, which indicates a high informativeness of the spectral data regarding this parameter. The refractive index after the initial stage of adaptation demonstrates a stable approximation to the real trajectory and correctly reproduces its trend, maintaining a small systematic lag caused by noise filtering. The absorption coefficient is characterized by slower convergence dynamics and increased sensitivity to random disturbances, however, in the long term it also demonstrates a direction of change consistent with the experiment. In conclusion, the results confirm the ability of the developed hybrid architecture to provide stable tracking of the evolution of the physical parameters of the material in real time without the need for repeated complete retraining of the model.

Parametric identifiability and uncertainty of coefficients. To assess the parametric identifiability of the system, an analysis of the local sensitivity of the spectral response of the "air–film–glass" structure to the parameters of the film thickness d, the refractive index n, and the absorption coefficient k was performed. The sensitivity was calculated numerically as the derivative of the reflection spectrum with respect to the corresponding parameter in the wavelength range 400-800 nm. The results obtained, shown in Fig. 8, show that the spectrum has the greatest sensitivity to changes in the film thickness, somewhat less to the refractive index, while the effect of the absorption coefficient is much weaker, i.e. $|S_d| > |S_n| > |S_k|$. This explains the slower and noisier convergence of the estimates of the parameter k during online adaptation of the digital spectral twin.

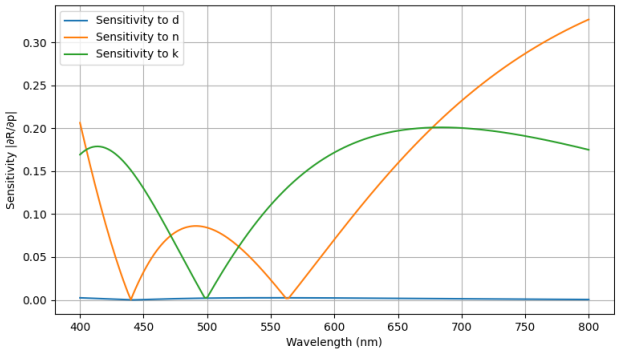

Fig. 8. **Local sensitivity of the reflection spectrum to film parameters**
***Source*: compiled by the authors**

The zero values of local sensitivity at some spectral points, shown in Fig. 8, are due to the interference nature of the reflection of thin films. At points where the spectrum has a local maximum or minimum, $\partial R/\partial\lambda \approx 0$ holds and changing the parameters has almost no effect on R. Therefore, the derivative can approach zero. This happens periodically due to interference.

To investigate the uncertainty of the coefficients, an ablation experiment was conducted to evaluate the influence of the parameter

stabilization mechanism during online adaptation. The results are presented in Table 3. We see that the use of the stabilization term reduces the *RMSE* by approximately 30-40 % at increased noise levels and provides more stable convergence of parameter estimates. In particular, at a noise level of 5 %, the *RMSE* value decreases from 0.094 to 0.057, and the parameter estimates demonstrate significantly more stable convergence without noticeable drift.

Accuracy and quality of work. For the obtained numerical data, the quality of the digital spectral twin was evaluated by the speed of convergence of the estimated parameters with the true values, the level of the root mean square error between the model and experimental spectra, as well as the time of the system entering the stable adaptation mode.

The following formula was used to calculate *RMSE*

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(S_{\exp}(\lambda_i) - S^*(\lambda_i))} .$$

This metric allows us to objectively assess the degree of agreement between the experimental and reconstructed spectra across the entire spectral range. Table 4 shows the generalized performance indicators of the system.

According to the results of numerical experiments, it is found that after the initial transition stage, the parameters of thickness, refractive index and absorption coefficient reach an average relative error of approximately 2.2 %, 0.8 % and 3.6 %, respectively, while the spectral approximation error is about 5.6 % with *RMSE*≈0.042. The obtained results indicate a stable convergence of the algorithm and effective tracking of slow drift of parameters in the long-term regime.

Testing on experimental data. In experimental works [32], [33], [34], a study of overvoltage nanosecond discharges in air, nitrogen and metal vapors was conducted, with the registration of plasma emission spectra emitted in a wide spectral range. The spectra obtained in these works contain line overlaps, noise components and a complex multicomponent structure, which in turn requires theoretical justification. Therefore, these experimental data are suitable for testing the developed hybrid system.

To experimentally verify the system's performance, the emission spectrum of a pulsed discharge plasma between tungsten electrodes [34] at atmospheric pressure (101 kPa) and an interelectrode distance of 2 mm was used. The experimental data contain 22 identified spectral lines of W I, N I, N II, O I and hydrogen atoms in the range of 330-1000 nm. Based on these values, an experimental spectral profile was constructed, which was used as a test set to verify the neural network module.

The system reconstructs the spectrum as a superposition of spectral lines, reproducing the positions of the main maxima and relative intensities for the dominant transitions W I and N II. To demonstrate the possibilities of selective approximation, the oxygen lines O I were not taken into account in the reconstructed spectrum. A comparison of the spectra, which is shown in Fig. 9, shows that the system correctly reproduces the main

Table 3. **Results of the ablation experiment**

Algorithm mode	**Noise level**	***RMSE***	**Stability of estimates**
Without stabilization	0 %	0.083	unstable parameter estimates
With stabilization	0 %	0.051	stable convergence
Without stabilization	2 %	0.062	notable fluctuations
With stabilization	2 %	0.048	stable convergence
Without stabilization	5 %	0.094	significant parameter drift
With stabilization	5 %	0.057	controlled drift

***Source*: compiled by the authors**

Table 4. **Generalized indicators of system performance**

Indicator	**Thickness *d***	**Indicator *n***	**Coefficient *k***	**Spectra *S*(*λ*)**
Stabilization time, iterations	≈80-100	≈120-150	≈150-180	≈220
Average relative error, %	≈2,2	≈0,8	≈3,6	≈5,6
RMSE after stabilization	≤0,025	≤0,012	≤0,001	≈0,042
Nature of adaptation	Ambulance	Stable	Slower	Stand

***Source*: compiled by the authors**

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structure of the spectrum, while the missing components appear only in the experimental profile. This confirms the ability of the hybrid system to work with real spectral data and perform their parametric reconstruction. The accuracy of the reproduction of the experimental spectrum was assessed by comparing the positions of the maxima and relative intensities of the spectral lines. The average deviation of the peak positions was about 0.12-0.18 nm, and the average relative error of the reproduction of intensities did not exceed 6-8 %, which indicates sufficient accuracy of the reconstruction of the spectral structure. At the same time, the *RMSE* of the normalized intensities was about 0.05, and the correlation coefficient between the experimental and reconstructed spectra exceeded 0.97, which indicates a high agreement of the results with the experimental data.

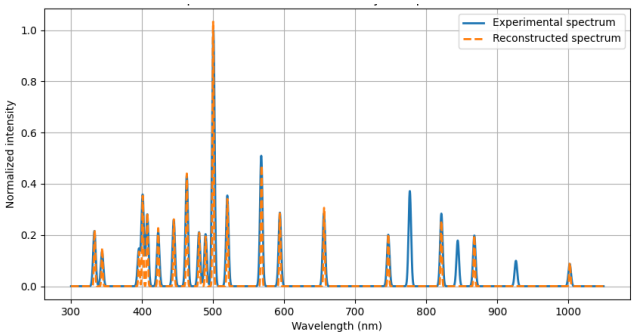

Fig. 9. **Comparison of experimental and reconstructed spectra**
***Source*: compiled by the authors**

Therefore, the use of a digital twin system allows you to simulate the plasma spectrum without repeating a complex experiment, providing reliable control over the parameters and generating test data for the neural network module, which significantly speeds up the verification of spectrum reconstruction algorithms and the assessment of their accuracy in reproducing key spectral characteristics.

Discussion of results. The results obtained confirm the effectiveness of the developed architecture of the digital spectral twin, built on a combination of a physical model and a neural network module. The formalization of the process of spectrum formation and parameter updating, presented in formulas (1)-(3), ensured consistency between experimental and model data, which is clearly demonstrated in Fig. 3, Fig.4, Fig. 5 and Fig. 6. The use of a physically based model of electromagnetic wave propagation in the "air–film–glass" structure allowed to reduce the uncertainty of parameter estimation compared to empirical methods, which is consistent with the results of works [23], [24]. The online adaptation mechanism described in formulas (4)-(5) ensures a gradual convergence of the estimated parameter values with the true ones in the process of a long experiment, which is reflected in Fig. 2, Fig. 3 and Fig. 4. This corresponds to modern trends in the integration of physics and machine learning, similarly to [25]. Analysis of the mean square error of the spectra indicates a stable decrease in the discrepancy between the experimental and reproduced data during adaptation (Fig. 7), which confirms the effectiveness of the self-learning mechanism and compensation of parametric drift. Unlike classical inversion methods used in nanophotonic design and spectral synthesis problems [21], the developed architecture provides dynamic adjustment of the solution in real time. Comparison with the concepts of digital twins presented in the works [26], [28, [29] shows the correspondence of the developed system to the modern idea of adaptive closed information models with constant updating based on experimental data. At the same time, the focus on spectroscopic identification of materials expands the scope of application of the developed concept.

Thus, the results of numerical experiments shown in Fig. 3, Fig. 4, Fig. 5 and Fig. 6 confirm that the integration of the physical model, the neural network approximator, and the self-adaptation module provides high accuracy of spectrum reproduction and stable identification of parameters under conditions of noise and parametric drift, which makes the architecture promising for the development of intelligent spectroscopic systems.

The scientific novelty of the work lies in the development of a hybrid information architecture of a digital spectral twin of a material system, which combines physically based methods of modeling optical processes with neural network algorithms of adaptive approximation and online self-learning mechanisms. Unlike existing methods, the work implements a closed loop of self-adaptation, within which the parameters of the physical model and the weights of the neural network are automatically adjusted based on the analysis of experimental spectral data in real time. This provides not only the reproduction of spectral characteristics, but also dynamic tracking of the slow drift of the physical parameters of the material, which is fundamentally important for practical applications.

The uniqueness of the work lies in the integration of TMM, RCWA and FEM methods with physically constrained neural network models within a single digital twin information system focused on spectral identification of materials. The developed architecture

combines modeling, identification, optimization and error control modules into a single adaptive loop, which ensures continuous model updating in accordance with current experimental conditions.

The main advantage of the developed architecture is the increase in the accuracy and stability of parameter identification due to the use of physical constraints in the process of neural network training and optimization. The neural network module allows to significantly reduce computational costs compared to direct numerical modeling, which ensures the possibility of system operation in real time. The closed loop adaptation helps to compensate for the influence of noise, instability of measuring equipment and slow changes in material properties. An additional advantage is the ability to visualize the evolution of spectra and parameters, which increases the interpretability of the results and the convenience of practical use of the system.

However, the developed system has certain limitations. The quality of the digital twin's operation largely depends on the accuracy of the experimental data, the correctness of the initial parameterization of the physical model, and the stability of the neural network training process. The implementation requires significant computational and software resources, as well as careful tuning of the adaptation parameters. In addition, at this stage, the system has been tested on artificial data for a limited class of thin-film structures, which requires further expansion of the experimental base.

Prospects for further research are related to the expansion of the developed system architecture to multilayer, nonlinear and functionally gradient materials, the integration of more complex PINN architectures, the automation of the selection of training parameters and model structure, as well as the creation of distributed and cloud platforms for scalable spectral monitoring. Further development of the system also involves its adaptation to the tasks of predicting material degradation, optimizing technological processes and building intelligent decision support systems in materials science and optoelectronics.

CONCLUSIONS

The work developed a hybrid architecture of a digital spectral twin system based on a physical model and a neural network module for identifying thin film parameters. Numerical experiments on artificially generated data in the range of 400-800 nm for a duration of 500 iterations showed a stable convergence of the estimated parameters with the true values in the presence of noise up to 1 % and parametric drift. The implemented online adaptation mechanism ensures a reduction in the mean square error of spectrum reproduction during the training process and achievement of a stable mode of operation of the digital twin during the first 100-200 iterations, and of the spectrum as a whole – up to 300 iterations. The error in estimating the film thickness does not exceed 2-3 %, the refractive index is about 0.05 %, and the absorption coefficient is less than 0.5 %, which indicates a high accuracy of parameter identification.

The work analyzes the parametric identifiability of the system based on the local sensitivity of the reflection spectrum to the film parameters, which allows us to establish the sensitivity ratio $|S_d|>|S_n|>|S_k|$ and explain the features of the convergence of estimates during online adaptation. In addition, an ablation experiment was performed, which showed that the use of the stabilization mechanism reduces the *RMSE* by approximately 30-40 % and provides a more stable convergence of the parameters of the digital spectral twin even in the presence of measurement noise.

Testing of the system on experimental data showed that the developed digital twin is able to accurately reproduce the positions of the main spectral maxima lines, their relative intensities and provide selective approximation. The average deviation of the peak positions was about 0.12-0.18 nm, and the average relative error of intensities reproduction did not exceed 6–8%, which indicates sufficient accuracy of the reconstruction of the spectral structure.

It is shown that the integration of physical constraints increases the accuracy and stability of the solution of inverse problems compared to classical offline inversion methods and allows for real-time parameter correction without repeated retraining of the model. The results obtained confirm the effectiveness of the developed architecture for automated spectroscopic analysis and its prospects for application in monitoring and optimization systems for thin-film technologies.

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Архітектура та реалізація гібридної системи прототипу цифрового спектрального двійника тонких плівок

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АНОТАЦІЯ

Актуальність зумовлена потребою створення інтелектуальних інформаційних систем для обробки спектроскопічних даних та ідентифікації параметрів матеріалів у режимі реального часу. **Метою** роботи є розробка гібридної архітектури прототипу цифрового спектрального двійника для ідентифікації параметрів тонких плівок у режимі реального часу. Для досягнення мети вирішено **завдання** інтеграції фізичних і нейромережевих моделей, реалізації механізму онлайн-самоадаптації та оцінювання ефективності системи на експериментальних даних. Реалізовано чисельну схему на основі **методу** матриці передачі та фізично-інформованих нейронних мереж для моделювання спектральних відгуків і адаптивного оцінювання параметрів. Досліджено механізм онлайн-самоадаптації, який безперервно оновлює параметри матеріалу на основі експериментальних спектральних даних за наявності шуму та повільного дрейфу, а також аналіз параметричної ідентифікованості на основі локальної чутливості спектра. **Результатом** роботи є розробка архітектури, що забезпечує стабільну збіжність оцінок товщини, показника заломлення та коефіцієнта поглинання протягом 100–200 ітерацій, а спектра в цілому – до 300 ітерацій. Досягнуто відносних похибок менше трьох відсотків для товщини, сотих відсотка для показника заломлення та десятих відсотка для коефіцієнта поглинання. Продемонстровано здатність моделі відстежувати поступові зміни параметрів, підтримувати високу точність прогнозування в довготривалому режимі та зменшувати похибку відтворення спектрів. Підтверджено стійкість до шуму та нестаціонарних умов, а також здатність точно відтворювати спектральні максимуми, відносні інтенсивності та забезпечувати селективну апроксимацію. Розроблена гібридна архітектура є ефективним інструментом інтелектуального спектроскопічного моніторингу та матеріалознавчої ідентифікації. Подальші дослідження будуть спрямовані на розширення системи для багатошарових структур і промислових вимірювальних систем.

Ключові слова: цифровий двійник; спектроскопія, гібридна інформаційна система; тонкоплівкові структури; нейронні мережі; ідентифікація параметрів; самоадаптація; оптичні властивості матеріалів

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