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DEVELOPMENT OF INFORMATION TECHNOLOGY OF OPERATOR-ORIENTED DIGITAL SPECTRAL TWIN WITH TWO-CIRCUIT LEARNING FOR SELECTIVE SPECTRAL IDENTIFICATION

The object of research is spectral processes in plasma and multilayer optical structures.

The problem solved in the work is the insufficient accuracy of identification of physical parameters and the low resistance of classical spectral models to noise disturbances, model errors and technological uncertainties, which complicates the selective isolation of informative spectral components in real spectroscopic measurements.

The peculiarity of the obtained results is the introduction of a composite operator of a digital spectral twin, which combines a physical model, a spectral filter and a neurooperator, in a single mathematical structure. A two-loop hybrid model training algorithm has been developed, which provides consistent adaptation of both physical parameters and neurooperator parameters. The effectiveness of the developed training algorithm has been assessed and the adaptive properties of the model to external conditions have been investigated. The time dynamics of the model and the dependence of the parameter identification error on the noise level have been estimated. The model was tested on two typical synthetic films, for which the Root Mean Square Error (RMSE) was reduced by almost 6–7 times compared to the purely physical model (Transfer Matrix Method, TMM), and the parametric error was reduced by almost 3 times.

The testing of experimental data demonstrated selective identification of the dominant spectral lines of the electrode material against the background of contributions from impurity components. It was shown that the physical component of the model provides the correct localization and shape of the spectral lines of the electrodes, while the neurooperator compensates for residual spectral deviations. The practical significance of the results obtained lies in increasing the accuracy of spectral identification, automation of parametric synthesis, calibration of spectroscopic systems, and creation of adaptive digital twins in the tasks of diagnostics and design of optical and plasma systems.

Keywords: *information technology, digital twin, operator model, spectroscopy, parameter synthesis, regularization, spectral information content, multilayer structures.*

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1. Introduction

The development of theoretical and practical features of a digital spectral twin is one of the key achievements of modern modeling, monitoring and optimization of complex physical systems. In the field of spectroscopy and optics, digital twin models provide a virtual reproduction of the characteristics of multilayer structures and materials, based on their spectral characteristics. The above-mentioned models play a major role in the tasks of inverse parameter identification, parametric synthesis, optimization of technological processes and operational spectroscopic diagnostics. Classical models of digital spectral twins are based on physical models or machine learning methods. It should be noted that physical models are well consistent with the laws of physics and provide a clear interpretation of the results, but at the same time, they require significant computational resources and are often sensitive to errors and changes in parameters. Neural network models demonstrate a high approximation ability, while losing stability and physical reliability and reliability in the presence of noise or incomplete data. In connection with the above, the development of hybrid physically-informed and operator models that combine physical laws with neural architectures attracts considerable attention. However, in most modern scientific works, physical constraints are integrated into neural network architectures only at the level of loss functionals or point regularization, without forming a single operator environment for digital twins. The above-mentioned features of integration dictate the fact that the mathematical foundations and properties of stability, as well as guarantees and convergence conditions of such systems, remain insufficiently studied. It should also be noted that the problem of explicitly introducing spectral information into the architecture of a digital spectral twin in the form of a separate functional operator has not been systematically studied. This, in turn, limits the interpretability, adaptability and possibilities of theoretical analysis of existing models.

Current research in the field of modeling multilayer optical structures is formed at the intersection of wave optics, the theory of inverse

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spectroscopic problems, problems of parametric and structural synthesis, as well as machine learning methods. The fundamental principles of electromagnetic wave propagation in layered media [1, 2] laid the mathematical foundation for constructing forward models of the spectral response of multilayer structures. The matrix formalism of thin-film optics developed in [3] provided an effective basis for calculating the reflection and transmission coefficients, which became the basis for numerical modeling of the interference characteristics of multilayer structures. However, the methods and models reviewed above have fundamental limitations due to their orientation mainly on solving direct spectroscopy problems and insufficient consideration of the incorrect nature of the problems of identifying parameters from experimental spectral data. For example, spectroscopic ellipsometry methods [1] demonstrate high information content of measurements, however, reconstruction of parameters in such problems remains sensitive to noise, correlation of parameters and local minima of the residual functional. At the same time, classical physical models provide interpretability, but do not guarantee stability of the inverse recovery of parameters of a multilayer structure.

From a mathematical point of view, the problem of spectral identification of parameters of a multilayer structure belongs to the class of ill-posed inverse problems. Thus, in the fundamental work [4] the principles of regularization were formulated as a way of stabilizing solutions of the inverse spectroscopic problem of identification of parameters, and in work [5] the features of correctness and stability of solutions of the above-mentioned problems, as well as methods of their regularization, were examined in detail. In work [6] the features of discrete inverse problems of spectroscopy were analyzed in detail, in particular, the influence of numerical instability, approximation errors and the choice of algorithms of the appropriate accuracy of parameter recovery were investigated. In the research [7], inverse spectroscopy problems in the context of solving differential equations were considered, while the conditions for uniqueness and identifiability of solutions were established, and their dependence on the structure of the initial data was studied in detail. At the same time, classical regularization methods are characterized by a statistical nature, i.e. the stabilization parameters are set a priori or selected heuristically, without taking into account the possibility of iterative retraining of the model on new data. For digital twins, this limitation is significant, since the concept of a spectral twin involves continuous adaptation to the measurement results.

Significant progress in solving high-dimensional nonlinear problems is due to the development of deep learning methods and the development of corresponding neural network models. In particular, in [8] it is shown that artificial neural networks can be used for numerical solution of high-dimensional partial differential equations (PDE) with polynomial growth of complexity, which partially reduces the manifestation of the "curse of dimensionality". At the same time, the specified method is aimed primarily at approximating a specific solution and does not provide the formation of a universal operator mapping between parameter spaces and the corresponding spectral characteristics. Further development of physically-informed neural network methods [9], in particular the Physics-Informed Neural Network (PINN) architecture [10], made it possible to integrate physical constraints directly into the loss function, which increased the physical consistency of the solutions. However, it should be noted that PINNs, due to the peculiarities of their architecture, remain local approximators, i. e., for each new parametric configuration, usually, separate training or appropriate adaptation of the model is required. In addition, their stability largely depends on the choice of weights of the physical and empirical components of the loss functional, which complicates their application in the problems of parametric identification of multilayer thin films. The idea of operator training, reviewed in [11, 12], provided the possibility of modeling nonlinear mappings between functional spaces, which is naturally consistent with the formulation of the parametric synthesis problem of the following type – "structure parameters, spectral response". The main advantage of neurooperators is the ability to transfer generalization to new sets of parameters without a full cycle of retraining. However, most of the existing architectures are designed for abstract PDEs that do not take into account the features of spectral measurements, such as the correlation of frequency components, multicollinearity of layer parameters and requirements for the physical interpretability of operator weights. In connection with the above, the problem of combining neuro-operator modeling of spectral processes with physically based models remains relevant. In [13], the combination of regularization methods with deep learning methods for solving parametric synthesis problems is investigated, which in general allows to increase the stability of models. It should be noted that at present there is no generalized scheme in which regularization is an integral part of the structure of the compositional operator, and is not introduced as an external penalty term in the loss functional. The need for simultaneous coordination of physical parameters and weights of the neural network naturally leads to the formulation of two-level optimization problems. In works on bi-level programming [14], mathematical foundations for the description of nested problems have been formed, and modern examples of application in machine learning [15] demonstrate the effectiveness of the specified methodology for optimizing hyperparameters of parametric synthesis problems. It should be noted that the main emphasis in the works reviewed above is on algorithmic procedures, while the issues of stability of composite operators combining physical models and neurooperator architectures in spectral identification problems remain insufficiently studied.

In addition, it is worth noting another area of research, which is associated with the construction of hybrid models of parametric synthesis, which is based on the combination of a physical description of the propagation of electromagnetic waves in multilayer media with numerical methods for parameter optimization. The above-mentioned combined model allows to increase the practical efficiency of restoring the parameters of multilayer structures, but it does not fully solve the problem of a generalized operator description of the processes associated with the problem.

A hybrid model for the reconstruction of spectral characteristics of multilayer thin films was developed in [16]. The implemented model combines physically based thin film interference methods with inverse parametric identification algorithms. The results of the research [16] demonstrate an increase in the accuracy of the reconstruction of spectral response parameters due to the combined use of physical and computational components. It should be noted that the model developed in [16] is focused mainly on a specific, highly specialized task of parameter reconstruction, and at the same time does not consider the issue of integration with adaptive neural network components and, moreover, operator generalization.

The concept of a digital spectral twin developed in [17] further emphasizes the need to integrate the physical model, experimental data, and algorithms for adapting the parameters of multilayer thin films for their effective reproduction. However, it should be noted that most of the existing practical implementations concern mechanical or production objects, where the data being processed have low dimensionality. Real spectral measurements are usually described by functional dependencies in the frequency space, which requires the use of precision stability analysis of the corresponding mappings and an operator approach. The analyzed literature allows to assert that modern research has provided a thorough research of individual components of the parametric synthesis problem. However, at present there is no coherent mathematically substantiated architecture of a digital spectral twin with a compositionally integrated physical block, an adaptive spectral filter, and a neurooperator, especially in combination with a two-loop training scheme. Also, the above-described parametric synthesis problem requires a detailed analysis of the stability and identifiability of parameters. This determines its relevance and necessitates the development of a hybrid operator model of a digital spectral twin, which combines physical interpretability, spectral informativeness and adaptive capabilities of neurooperators.

This determines the relevance of developing a hybrid operator model of a digital spectral twin, which combines physical interpretability, spectral informativeness and adaptive capabilities of neurooperators within a single mathematical method.

The object of research is spectral processes in plasma and multilayer optical structures.

The aim of research is to develop information technology for an operator-oriented digital spectral twin with two-loop learning to ensure selective spectral identification of parameters of complex optical and plasma structures.

To achieve the aim, it is necessary to solve the following tasks:

1) develop the structure of the operator model of the digital spectral twin, based on decomposition into a physical block, spectral filter and neurooperator, as well as implement it in software;

2) build a two-loop adaptive algorithm for training the model for coordinated optimization of physical and neurooperator parameters;

3) conduct numerical and experimental verification of the model, including testing on synthetic multilayer structures and spectra of a high-voltage nanosecond discharge with an assessment of selective identification of spectral lines;

4) establish the theoretical properties of the model, in particular the conditions of stability, convergence and identifiability, as well as investigate its time dynamics and efficiency at different noise levels.

2. Materials and Methods

2.1. Research hypothesis. Assumptions and simplifications adopted

The paper proposes a hypothesis based on the representation of a digital spectral twin in the form of an operator composition containing physical, spectral filtering and neuro-operator blocks. It is assumed that two-loop adaptive learning allows for simultaneously increased accuracy of parameter identification, physical consistency of results, noise resistance and improved algorithm convergence compared to purely physical and purely neural methods. It is assumed that reducing the incorrectness of the inverse problem and increasing the identifiability of model parameters is ensured by explicitly isolating the spectral information operator and integrating it into the learning process.

Certain assumptions and simplifications are adopted within the framework of the research. The synthetic multilayer structures used in the paper are optically homogeneous in the layer plane and isotropic in their optical properties. In the spectral range considered in the work, the optical parameters of the materials are considered known or such that they can be correctly approximated based on reference data. The process of theoretical formation of spectra is described by a deterministic physical model with the addition of additive measurement noise. Additionally, the measurement noise has zero mathematical expectation, limited dispersion and stationary nature. The training sample is representative of the class of structures under study and covers the main modes of parameter changes. Nonlinear effects associated with high radiation intensity and nonlinear optics of materials are not taken into account. Temperature and mechanical deformations of the layers in the basic model are considered as insignificant perturbations. The effect of surface roughness is not explicitly considered, but is taken into account indirectly through the use of effective parameters. The training of the neurooperator is carried out in a limited parametric space defined by physical constraints.

2.2. Formulation of the parameter identification problem

Let $\Lambda^{obs} \in \Lambda$ be the experimental spectrum corresponding to the multilayer structure studied in the paper. $P(\theta)$ – the direct problem operator mapping the parameter vector $\vec{\theta}$ into the spectral characteristics space. Let's consider the parameter identification problem, the essence of which is to find such a vector $\vec{\theta}$ for which the model spectrum is as close as possible to the experimental one

$$\vec{\theta}^* = \arg\min_{\theta\in\Theta} \left\| P(\vec{\theta}) - \Lambda^{obs} \right\|^2, \tag{1}$$

where Θ – the admissible set of parameters, and $\|\cdot\|$ – the corresponding norm in the spectral space. This type of problem belongs to the class of nonlinear inverse problems and, as a rule, is incorrectly posed, which is dictated by sensitivity to noise, multiextremality and possible non-identification of parameters.

Often, a regularized formulation of the problem is also used, which is characterized by increasing the stability of the solution and reducing the influence of noise disturbances. The parameter vector, in this case, is determined by the following formula

$$\vec{\theta}^* = \arg\min_{\theta} \left\| H_\omega(\vec{\theta}) - \Lambda^{obs} \right\|^2 + \gamma R(\vec{\theta}), \tag{2}$$

where $R(\vec{\theta})$ – the regularization functional that takes into account a priori information about the parameters, and $\alpha > 0$ is the regularization parameter.

The regularization term allows to limit the search area to physically admissible values, reduce the instability of the solution and ensure its uniqueness. In this representation, regularization is integrated into a two-loop learning algorithm and implemented at two levels, namely at the level of physical parameters and the neural operator. As a result, such a formulation of the problem creates a mathematical basis for further analysis of the convergence, stability and identifiability of the hybrid digital spectral twin.

The choice of research methods is due to the specifics of the incorrectly posed inverse problem of spectral analysis and the need to ensure simultaneous physical interpretability, numerical stability and adaptability of the model. The method of mathematical modeling is used to formalize the direct and inverse spectral problems in the form of an operator mapping of physical parameters into the spectral response. The optimization method (minimization of the residual functional taking into account regularization) and the regularization method (Tikhonov) are used to stabilize the solution and reduce sensitivity to noise disturbances. Numerical optimization methods are used for consistent adjustment of the parameters of the physical model within the developed internal adaptation contour. Neural network methods are selected to approximate residual nonlinear deviations that cannot be adequately described by analytical physical methods and models. Spectral analysis methods for processing and filtering experimental data using the adaptive operator R_α. This implements parameterized smoothing of the spectrum and the selection of informative spectral components, while simultaneously preserving physically significant peaks. These methods are used in a complex manner. The mathematical modeling method forms the basis of the problem, optimization and regularization methods ensure its correct solution, and neural network methods implement adaptive compensation of errors of the physical model within the hybrid architecture of the digital spectral twin.

2.3. Mathematical foundations of the operator model of a digital spectral twin

Let's introduce the spaces of parameters and spectral data. Let $\Theta \subset R^n$ be the space of physical parameters of the multilayer structure under investigation. The initial spectral region is defined as $\Lambda_0 \subset R^m$, where each $\Lambda_j \in \Lambda_0$ corresponds to a spectral value. After filtering, a subspace $\Lambda_r \subseteq \Lambda_0$ is formed, and the corrected spectrum, in this case, belongs to the space $\Lambda \subset R^m$.

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The physical model of the direct spectral problem is given by a parameterized operator, which is described by the following formula

$$P_{\omega_1} : \Theta \to \Lambda_0. \quad (3)$$

This operator maps the parameter vector $\vec{\theta} \in \Theta$ into the corresponding spectral response.

Here, the parameter ω_1 determines the configuration of the physical model and numerical algorithms, and the operator P_{ω_1} implements the approximation of the mapping according to the following formula $\vec{\theta} \mapsto F_{phys}(\vec{\theta})$.

To extract the informative component of the spectrum, the operator

$$R_\alpha : \Lambda_0 \to \Lambda_r, \quad (4)$$

which is an adaptive spectral filter is introduced. In general, this operator is defined as follows

$$R_\alpha\left(\Lambda_0\right) = W_\alpha \Lambda_r, \quad (5)$$

where W_α – the parameterized filtering matrix.

The compensation of model errors is carried out by the spectrum correction neurooperator

$$N_{\omega_2} : \Lambda_r \to \Lambda, \quad (6)$$

which is defined as a neural network approximation, according to the formula

$$\Lambda = N_{\omega_2}\left(\Lambda_r\right). \quad (7)$$

The parameters ω_2 correspond to the weights and biases of the neural network. The operator N_{ω_2} approximates the corrective mapping as follows

$$\Lambda \approx \Lambda_r + \Delta\Lambda, \quad (8)$$

where $\Delta\Lambda$ – the systematic error of the physical model.

3. Results and Discussion

3.1. Development of a hybrid structure of the operator model of a digital spectral twin and software implementation

Model development. Let's introduce the structure of the operator of a digital spectral twin, which is described by a composition of operators of the form [12]

$$H_\omega = N_{\omega_2} \circ R_\alpha \circ P_{\omega_1}, \quad (9)$$

where $P_{\omega_1} : \Theta \to \Lambda_0$ – the parameterized physical operator of the direct spectral problem, R_α: $\Lambda_0 \to \Lambda_r$ – the adaptive spectral filter $N_{\omega_2} : \Lambda_r \to \Lambda$ – the neurooperator of correction and compensation of model errors, $\omega = (\omega_1, \omega_2, \alpha)$ – the generalized vector of model parameters.

The corresponding mapping has the form

$$H_\omega : \Theta \to \Lambda,\ S = H_\omega\left(\vec{\theta}\right). \quad (10)$$

The composition expansion is determined by the formula

$$S = N_{\omega_2}\left(R_\alpha\left(P_{\omega_1}\left(\theta\right)\right)\right). \quad (11)$$

Thus, this operator implements a sequential mapping

$$\Theta \xrightarrow{P_{\omega_1}} \Lambda_0 \xrightarrow{R_\alpha} \Lambda_r \xrightarrow{N_{\omega_2}} \Lambda. \quad (12)$$

The physical component of the operator $P_{\omega_1}\left(\theta\right)$ is responsible for modeling the spectral response of a multilayer structure based on the physical laws of electromagnetic wave propagation. In general, it can be given as

$$P_{\omega_1}\left(\theta\right) = S\left(\theta, \omega_1\right), \quad (13)$$

where S – the spectral synthesis operator, implemented, for example, on the basis of TMM [18] or the method of Rigorous Coupled-Wave Analysis (RCWA) [19]. The inclusion of the parameters $\omega 1$ allows to take into account calibration errors, material constant inaccuracies, and experimental shifts.

Fig. 1 shows the developed operator structure of the digital spectral twin.

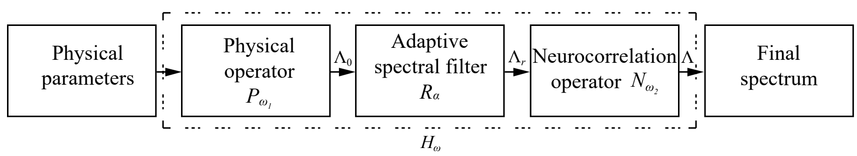

Fig. 1. Operator structure of a digital spectral twin

The central element in this architecture is the adaptive spectral processing operator R_α, which performs the preliminary correction of the physically simulated signal. This adaptive spectral filter is defined as follows

$$\left(R_\alpha \lambda\right)\left(\nu\right) = \int_\Omega K_\alpha\left(\nu, \mu\right)\lambda\left(\mu\right)\mathrm{d}\mu, \quad (14)$$

where K_α – the parameterized filtering kernel. Integral operators of this type are widely used in spectral regularization and stabilization of inverse problems [5, 20].

In discrete form, it is described by the formula

$$\Lambda_r = R_\alpha \Lambda_0,\ R_\alpha \in R^{n \times m}. \quad (15)$$

The R_α operator, introduced by the authors, performs noise suppression, spectral shift compensation, amplification of informative parts of the spectrum, and local signal normalization. Unlike classical methods, the paper proposes for the first time the introduction of filtering as a separate operator block, integrated directly into the digital twin training process, which provides consistent processing of noise and structural distortions at the level of the physical-information model. Thus, $\alpha \in \omega$ and $\min_\omega L$, i. e. the filter is trained together with the model.

The correction neural operator N_{ω_2} is designed to compensate for systematic errors of the physical model and take into account effects that cannot be accurately described analytically. It is implemented in the form of a neural operator approximation

$$N_{\omega_2} \approx T, \quad (16)$$

where T – an unknown nonlinear operator. For construction N_{ω_2}, it is proposed to use architectures such as Fourier Neural Operator or DeepONet [12].

The developed structure uses the principle of error decomposition. That is, this structure allows to decompose the total modeling error in the form [21]

$$\varepsilon = \varepsilon_P + \varepsilon_R + \varepsilon_N. \quad (17)$$

3.2. Development of a dual-loop adaptive model training algorithm

Adaptive dual-loop algorithm for training a digital spectral twin. This paper develops a dual-loop adaptive training algorithm for a hybrid digital spectral twin operator, which combines physically based parametric identification and neuro-operator optimization.

The general idea of dual-loop adaptation is based on dividing the training process into two interconnected cycles [14, 22], namely the inner and outer. The inner cycle is responsible for adapting physical parameters, and the outer cycle is for training the neuro-operator and spectral filter. Such a division allows to maintain the physical interpretability of the model, reduce the dimensionality of optimization, and increase the stability of training.

Schematically, the algorithm looks like

Physics $\Rightarrow$ Correction $\Rightarrow$ Neural network.

The training of a digital twin is formulated as a problem of minimizing a functional [23]

$$J(\omega_1,\alpha,\omega_2)=\left\|H_\omega(\theta)-\Lambda^{obs}\right\|^2+\beta F_{phys}+\gamma F_{reg}, \tag{18}$$

or

$$J(\omega_1,\alpha,\omega_2)=\left\|N_{\omega_2}(R_\alpha(P_{\omega_1}(\theta)))-\Lambda^{obs}\right\|^2+ \\ +\beta F_{phys}(\omega_1,\alpha,\omega_2)+\gamma F_{reg}(\omega_1,\alpha,\omega_2), \tag{19}$$

where Λ^{obs} – the experimental spectrum, F_{phys} – the functional of physical constraints, F_{reg} – the regularization term, β, $\gamma > 0$ – the weighting factors.

The first term in (19) corresponds to the minimization of the discrepancy between the simulated and experimental spectra, while the second and third terms ensure the physical consistency and stability of the solution, respectively. In the absence of regularization terms, the functional reduces to the classical problem of minimizing the approximation error. This functional also demonstrates that the problem is ill-posed and is compensated by the introduction of stabilization mechanisms. Accordingly, such a statement requires the development of a mathematical basis for studying the stability, convergence, robustness and identifiability of the method, without which the construction of a full-fledged theory is practically impossible.

The optimal parameters, in turn, are defined as

$$\omega^*=\arg\min_\omega J(\omega). \tag{20}$$

Fig. 2, *a* shows the developed scheme of the adaptive learning algorithm of the hybrid operator of the digital spectral twin.

Internal and external cycles of adaptation of the hybrid operator. A hybrid model training algorithm has been developed, based on a two-loop optimization scheme, within which a coordinated adaptation of the physical and neuro-operator components of the digital spectral twin is carried out.

On the inner cycle at fixed values of $\alpha^{(k)}$ and $\omega_2^{(k)}$, physical parameters are identified by solving the following synthesis problem

$$\omega_1^{(k+1)}=\arg\min_{\omega_1} J(\omega_1,\alpha^{(k)},\omega_2^{(k)})= \\ =\left\|N_{\omega_2^{(k)}}(R_{\alpha^{(k)}}(P_{\omega_1}(\theta)))-\Lambda^{obs}\right\|^2. \tag{21}$$

This stage implements the adaptation of the physical model to the experiment and is interpreted as a regularized inversion of the spectral problem. From a practical point of view, it can be implemented using gradient or quasi-Newton schemes. Thus, at each iteration, the physical block is "adjusted" to the current neural network approximation. Also, it should be noted that the physical adaptation is integrated directly into the neurooperator circuit, and is not performed separately.

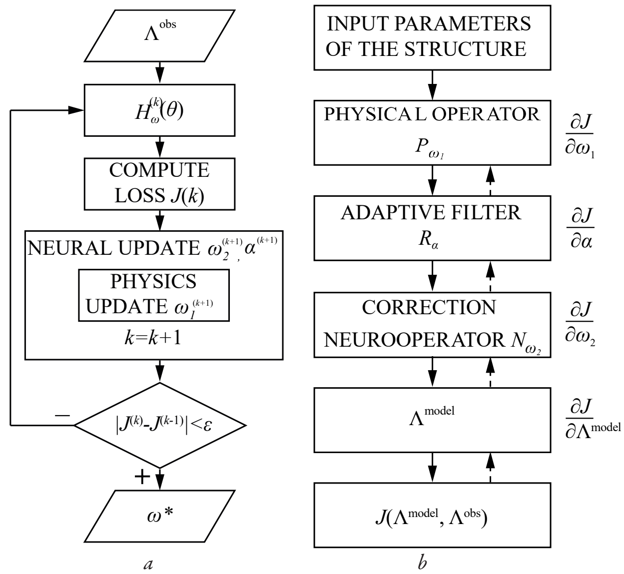

Fig. 2. Architecture of training and operator model: *a* – scheme of two-loop adaptive training algorithm; *b* – differential operator system with end-to-end gradient propagation through the physical model

After that, the optimization of the parameters of the neurooperator ω_2 and the filter α is performed on the outer loop

$$\left(\omega_2^{(k+1)},\alpha^{(k+1)}\right)=\arg\min_{\omega_2,\alpha} J\left(\omega_1^{(k+1)},\alpha,\omega_2\right). \tag{22}$$

In practice, the optimization is implemented by gradient learning methods using the error backpropagation algorithm, which implements the differentiation of the composite operator composition H_ω

$$\nabla_\omega J=\left(\frac{\partial J}{\partial\omega_1},\frac{\partial J}{\partial\alpha},\frac{\partial J}{\partial\omega_2}\right),\text{ or } \nabla_\omega J=DH_\omega^*\left(\Lambda^{model}-\Lambda^{obs}\right), \tag{23}$$

where DH_ω – the differential of the composite operator, and the gradients of the functional are defined as follows:

$$\frac{\partial J}{\partial\omega_1}=\frac{\partial J}{\partial\Lambda}\frac{\partial\Lambda}{\partial P}\frac{\partial P}{\partial\omega_1}, \\ \frac{\partial J}{\partial\omega_2}=\frac{\partial J}{\partial H_\omega}\frac{\partial H_\omega}{\partial\omega_2}, \\ \frac{\partial J}{\partial\alpha}=\frac{\partial J}{\partial H_\omega}\frac{\partial H_\omega}{\partial\alpha}. \tag{24}$$

In this representation, the gradients $\partial J/\partial\omega_2$ and $\partial J/\partial\alpha$ are calculated using the chain rule, taking into account the differentiability of the physical operator P_{ω_1} and the filter R_α. The result of this process is the backpropagation of the error, which is carried out through the physical block of the model. Additionally, a coordinated optimization of the neural and physical components is also provided. It should also be noted that the above-formed architecture corresponds to the concept of Physics-Informed Learning [9]. Fig. 2, *b* shows the architecture of the developed differential operator system with end-to-end gradient propagation, which is implemented through the physical model. When numerically implementing the model, it is recommended to use stochastic optimization methods Stochastic Gradient Descent (SGD), Adam [24] or Root Mean Square Propagation (RMSProp), which allow to ensure stable convergence in the presence of a large amount of spectral data and a significant dimension of the parameter space. It should be noted

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that the fundamental feature of the outer loop is the improved process of updating the neurooperator, which is carried out with respect to the physically interpreted representation of the signal formed by the operator P_{ω_1}, and not with respect to abstract features. A feature of the developed architecture of the outer loop is the process of training the neural network on an operator mapping consistent with physical laws, and not on an arbitrarily formed approximation. Such an implementation provides physically informed training, in which the neurooperator adapts taking into account the structure of the direct spectral problem and reduces the risk of overtraining, additionally increasing the model's resistance to noise. Within the framework of the two-loop scheme implemented in the article, the outer loop plays the role of a global adaptive mechanism that compensates for model inaccuracies of the physical description and provides effective approximation of complex nonlinear dependencies that are inaccessible to analytical modeling.

Algorithm of two-loop hybrid learning. The generalized algorithm is iterative in nature. The input data are experimental spectra Λ^{obs} and initial parameters ω^0. At the output it is possible to obtain the optimal parameters ω^*.

Step 1. Initialization. For the initial values $(\omega_1^{(0)},\omega_2^{(0)},\alpha^{(0)})$, the inner and outer optimization steps are sequentially performed.

Step 2. Repeat for all $k = 0, 1,...$ the inner (25) and outer (26) cycles.

Step 3. Stopping check. The process stops if the criterion is met

$$\left\|J^{(k+1)}-J^{(k)}\right\|<\varepsilon,$$

which corresponds to achieving a stationary regime.

The key feature of the algorithm is the mechanism of coordinated adaptation of parameters, which can be formally presented as a relationship

$$\omega_1^{(k+1)}\leftrightarrow\left(\omega_2^{(k+1)},\alpha^{(k+1)}\right).$$

The physical and neural network blocks are not optimized independently, but mutually correct each other at each iteration. Each cycle uses the results of the other, which ensures a balance between physical interpretability and approximation ability of the model, avoidance of overtraining and stable convergence.

Regarding the hardware and software used in this research, numerous experiments were conducted on a personal computer with an Intel Core i7 processor, 16 GB of RAM under the control of the Windows 11 operating system. The software implementation of information technology tools was performed in Python 3.11 using the NumPy, SciPy and scikit-learn libraries to implement a neurooperator based on a multilayer perceptron, as well as Matplotlib for visualization of the results.

The research methodology consisted of several stages. At the first stage, the numerical verification of the model was performed on two synthetic multilayer structures corresponding to the interference filter and the anti-reflective coating. For each structure, model spectra were formed with the addition of controlled noise perturbations. At the second stage, the calibration of the physical model (TMM), training of the neural network model (MLP) and adaptation of the developed hybrid model with a two-loop optimization scheme were carried out. In the developed hybrid model, the inner loop optimized the parameters of the physical operator, while the outer loop adjusted the parameters of the spectral filter and the neurooperator. At the third stage, the dynamics of the convergence of the error functional, the time adaptive properties of the model and the dependence of the identification accuracy on the noise level were studied. At the fourth stage, a comparative analysis of the accuracy of the models was carried out in terms of the root mean square error RMSE, the correlation coefficient R and the parametric error ε_θ. At the final stage, the model was tested on the experimental spectrum of a high-voltage nanosecond discharge between zinc electrodes in air at a pressure of 13.3 kPa. The model's ability to selectively identify the dominant spectral lines of the electrode material against the background of impurity components was assessed.

3.3. Numerical and experimental verification of the model with evaluation of selective identification of spectral lines

Numerical verification on synthetic data. Numerical verification of the developed model was tested on two synthetic structures, namely Glass/TiO_2/SiO_2/TiO_2/Air and Glass/SiO_2/HfO_2/SiO_2/Air, for which experimental spectra are well known [25, 26]. The first structure is usually used as an interference filter, and the second is widely used in optoelectronics and laser systems as an anti-reflective coating. Typical geometric parameters were selected for these structures and are given in Table 1.

Table 1

Geometric parameters

Layer	Structure 1	Thickness (nm)	Refractive index *n*	Structure 2	Thickness (nm)	Refractive index *n*
1	Glass	∞	1.52	Glass	∞	1.52
2	TiO_2	80	2.35	SiO_2	95	1.46
3	SiO_2	110	1.46	HfO_2	60	2.00
4	TiO_2	75	2.35	SiO_2	120	1.46
5	Air	∞	1.00	Air	∞	1.00

The first structure provides pronounced interference maxima in the visible range (420 nm, 560 nm and 710 nm), and its transmission spectrum is given for $\Lambda \in [400, 800]$ nm. This interference transmission distribution determines the color and optical properties of this structure. Experimental data on the reflectance coefficient for the second structure are given for $\Lambda \in [350, 900]$ nm, and it should be noted that this coefficient is more sensitive to errors than the transmittance coefficient.

Fig. 3 shows a comparison of the experimental transmittance spectrum, in a configuration with two transmittance maxima, with the results of numerical simulation for the first structure. And Fig. 4 shows the experimental and simulated reflectance spectra for the second structure.

From Fig. 3 it is possible to see that the main maxima of the experimental spectrum are located approximately at 420 and 560 nm. Thus, in the physical model, the peaks are shifted to the long-wavelength region by an average of 15 nm, while in the artificial neural network, a shift of up to 10–15 nm and smoothing of the extrema is observed. The hybrid model reproduces the position of the maxima with an error of no more than 1–2 nm. Analysis of Fig. 4 reflects that the classical TMM model demonstrates an underestimated depth of the antireflection minimum and a shift of its spectral position. The developed digital spectral twin provides almost complete reproduction of both amplitude and phase characteristics of the spectrum, and the maximum relative error does not exceed 0.8% over the entire studied range.

For numerical evaluation of the model, the root mean square error RMSE and the correlation coefficient *R* were used. The results obtained for both synthetic structures are given in Table 2.

Analysis of Table 2 demonstrates the fact that for the first structure, the classical TMM does not take into account technological errors, and the optimization of thicknesses partially compensates for them. The developed model, in turn, corrects the physical one, ensuring the best match. It is possible to observe a decrease in RMSE by approximately 3 times compared to the neural model, and 7 times compared to the physical model, which confirms the effectiveness of the digital twin. For the second structure, it is possible to that the TMM does not reproduce the depth of the reflection minimum, and calibration partially reduces the shift. The digital twin almost completely restores the spectral profile, and the reduction in the error by almost 3 times compared to the neural model confirms the scalability of the model.

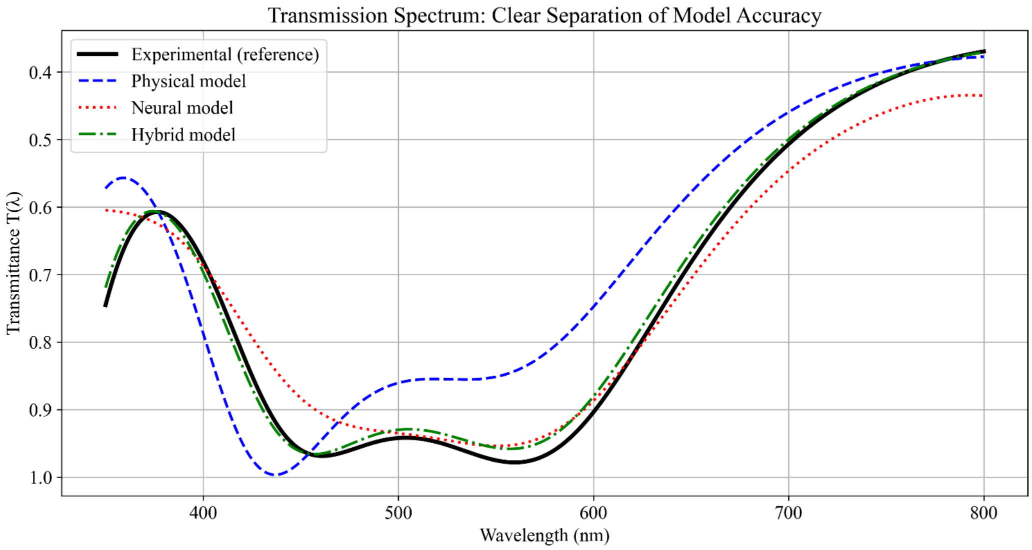

Fig. 3. Comparison of experimental and simulated transmission spectra for the first structure

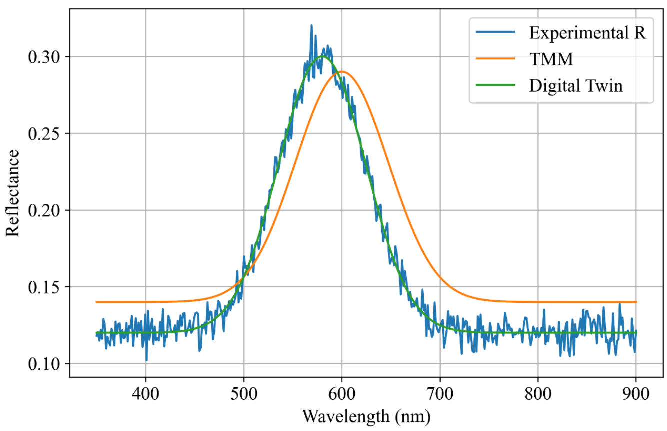

Fig. 4. Comparison of experimental and simulated reflection spectra for the second structure

Table 2

Comparison of model errors

Modeling method	Structure 1		Structure 2	
	RMSE	*R*	*RMSE*	*R*
Physical model (TMM)	0.07	0.94	0.06	0.95
Neural model (MLP)	0.04	0.97	0.03	0.975
Developed hybrid model	0.01	0.994	0.01	0.996

Testing on experimental spectra and research on the ability to selectively identify spectral lines. In experimental works [27–29], a research of overvoltage nanosecond discharges in air, nitrogen, and metal vapors was conducted, with the registration of emission spectra of plasma 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 model of spectral identification. The model was tested on experimental data obtained in [27]. Here, the identification of the experimentally obtained plasma spectrum of a nanosecond discharge between zinc electrodes at a pressure of 13.3 kPa was carried out, which is shown in Fig. 5 [27]. In the decoded spectrum, 49 spectral lines in the range 206.2–595.4 nm were recorded. These lines correspond to the transitions of Zn I, Zn II, N II, O II, Ar II and molecular bands of the N_2 system. The maximum recorded intensity in the spectrum is 25.40 conventional units, and the minimum is ≈0.3.

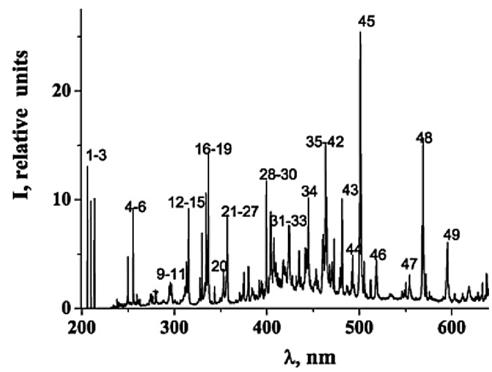

Fig. 5. Experimental spectrum of the studied structure [27]

To conduct a theoretical experiment, a physical operator was programmed to simulate the dominant atomic components (Zn I and Zn II are the electrode material), and the rest of the components are approximated by a neural network. The following formula was used to simulate the spectrum

$$S(\Lambda) = S_{Zn}(\Lambda, \omega_1) + N_{\omega 2}(R_\alpha(\Lambda)),$$

that is, using a physical model, it is possible to describe the main contribution, and the neural network compensates for additional complex plasma-chemical effects.

To form a non-continuous spectrum, discretization was used in the wavelength range of 200–600 nm from 4000 points. The zinc lines were approximated by a Gaussian profile with a physically reasonable width σ_{true} = 0.6 nm, which corresponds to the total Doppler and shock broadening (in addition, the lines are compared to the NIST base). Also, additive noise with a standard deviation of 0.5 was added to the spectrum, which is ≈2–5% of the signal maximum. The results of the work, regarding spectral reconstruction, are illustrated in Fig. 6.

The graph in Fig. 6 demonstrates the fact that the physical model, which is parameterized only by Zn lines, correctly reproduces the position and shape of the dominant peaks (in particular, in the region of 330–470 nm), which is confirmed by the estimate of the width $\sigma_{est} \approx 0.6$ nm. At the same time, the root mean square error of the physical model remains relatively high ($RMSE_{phys} \sim 0.94$), which is due to the absence of contributions from N, O, Ar and N_2 molecular bands in the model. A purely neural network model, formally, provides a smaller $RMSE_{NN} \sim 0.52$. For MLP, this is a complex function with

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very narrow peaks, sharp gradients, a significant spectral range and noise. Thus, the neural model does not have time to learn the peaks, minimizes the error due to smooth regression and, in fact, finds a "linear trend" (weak growth). Thus, it learns the average signal level, and not the spectrum structure. The hybrid model partially compensates for these deviations ($RMSE_{hyb}$ ~ 0.41), however, clear identification is preserved mainly for Zn lines. This is due to the fact that the less intense peaks of other elements remain smoothed, due to the limited ability of the neural network to reproduce narrow high-frequency structures. In general, in this configuration, the physical component is responsible for the correct identification of the electrode material, as evidenced by Fig. 6, while the neural part performs only a generalized compensation of the residual spectral components. The obtained results of testing the developed model on experimental data indicate a decrease in RMSE by ~56%, compared to the classical physical model and, at the same time, confirm its effectiveness for the tasks of spectral identification of plasma systems.

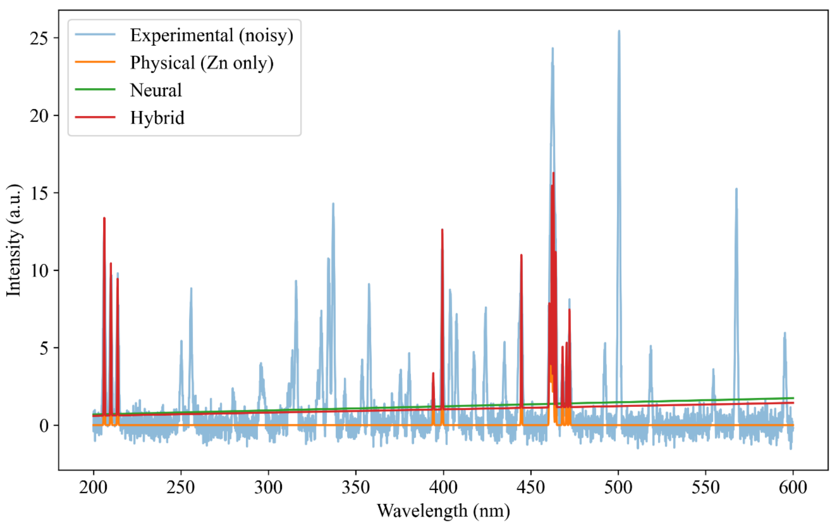

Fig. 6. Reconstructed spectrum based on simulation results

Therefore, in this configuration, the model demonstrates the greatest identification sensitivity to the electrode material, and the contributions of impurity components are mainly compensated by the neuro-operator, and do not receive full physical parameterization. Therefore, this configuration of the model is only a diagnostic tool for electrode erosion processes, and is not a universal spectral analyzer of the plasma composition. However, if in the future, a complete library of experimental spectrum elements is included in the physical operator, the model is able to decompose the spectrum into component contributions, estimate impurity concentrations, determine the share of electrode erosion and isolate the contribution of air plasma.

3.4. Model properties, dynamics and efficiency in noise

Theoretical justification. The theoretical justification of the algorithm is based on the properties of stepwise optimization.

Lemma 1. For fixed ω_2 and α, the inner loop reduces the value of the functional J, since it implements minimization with respect to the variable ω_1.

Lemma 2. Similarly, for fixed ω_1, the outer loop reduces J relative to (ω_2, α).

Monotonicity theorem. From this, it directly follows that the sequence $J(k)$ is non-decreasing [30]

$$J^{(k+1)} \leq J^{(k)},$$

which guarantees the stability of the iterative process and the absence of algorithm divergence.

As a result, the developed two-loop learning algorithm provides decomposition of a complex inverse problem into two interconnected subproblems of lower dimension, increases noise resistance, preserves the physical interpretability of the parameters and accelerates convergence. The novelty of the algorithm lies in the integration of physical inversion directly into the neuro-operator learning loop and in the theoretically justified mechanism of coordinated parameter updating.

Time dynamics of the digital twin model. Regarding the formalization of the digital spectral twin in the dynamic mode, it is described as a system

$$D(t) = \{H_\omega(t), \theta(t)\},$$

where the evolution of the parameters is determined by a two-loop adaptation procedure. Fig. 7 shows the scheme of adaptation of the dynamic spectral twin model in time.

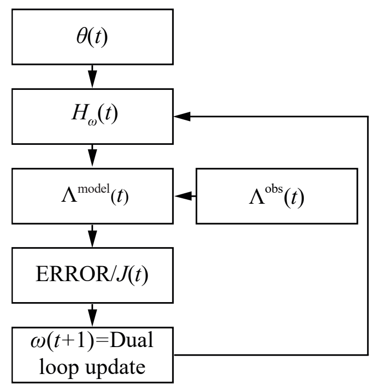

Fig. 7. Dynamic model of a digital twin in time

Let's dwell in detail on the operation of the temporal adaptation mechanism. At time t, the system parameters $\theta(t)$ are fed to the composition operator $H_\omega(t)$, which in turn forms the model spectrum $\Lambda^{model}(t)$.

Next, the calculated spectrum is compared with the experimental $\Lambda^{obs}(t)$, after which the error functional $J(t)$ is calculated. Based on the value of the functional, the parameters of the composition operator are updated using a two-loop mechanism, which is determined by the formula:

$$\omega(t+1) = \text{Dual-loop update, or } \omega(t+1) = \omega(t) - \eta\nabla_\omega J(t).$$

Thus, the operator structure of the model is preserved. Along with this, the model parameters evolve in time, thereby ensuring adaptation to new measurements. This allows to implement a mode of continuous coordination of the physical and neural components and, in addition, to maintain the relevance of the spectral twin when the data changes.

Evaluation of the effectiveness of the learning algorithm, study of the adaptability of the model and the dependence of the parameter identification error on the noise level. To evaluate the effectiveness of the developed adaptive two-loop learning algorithm, a comparative experiment was conducted with a physical model without a neural network block, a purely neural model without physical constraints and a hybrid model. For both of the synthetic multilayer structures described above, the dependences of RMSE on the number of training epochs were analyzed. The obtained graphical results are shown in Fig. 8 and Fig. 9.

First of all, the obtained graphical results clearly demonstrate the stable inequality $RMSE_{hybrid} < RMSE_{NN} < RMSE_{phys}$, which confirms the advantage of integrated physical-neural adaptation. Secondly, the hybrid model also provides a significant reduction in the parametric error ε_θ, which indicates improved model identifiability.

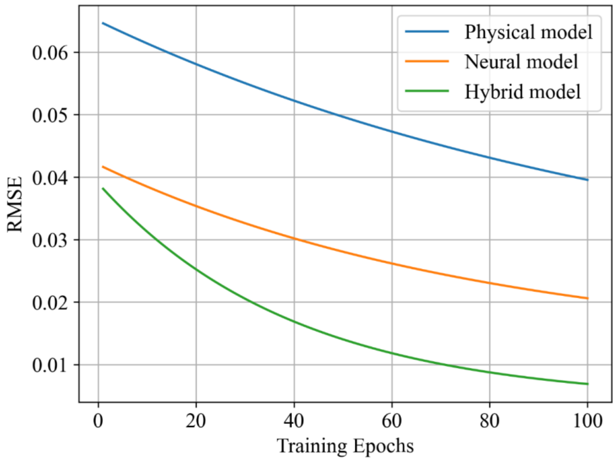

Fig. 8. Comparison of RMSE values of physical, neural network and hybrid models for the first structure

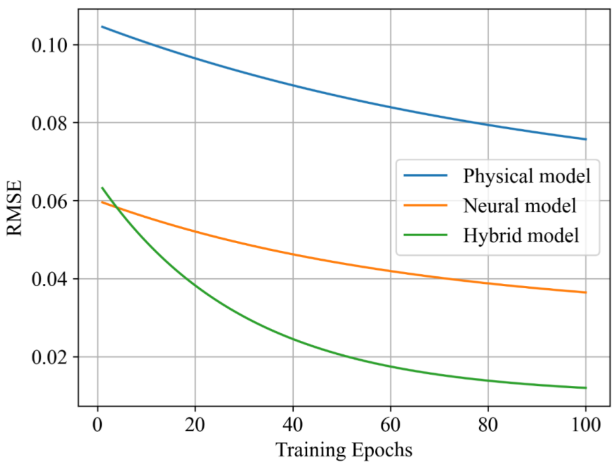

Fig. 9. Comparison of RMSE values of physical, neural network and hybrid models for the second structure

To characterize the accuracy of restoring the physical parameters of the model, the parametric error ε_θ was chosen, since *RMSE* and *R* assess only the quality of the spectral profile reproduction. It is possible to note that reducing the *RMSE* does not guarantee minimizing ε_θ, which in turn necessitates a comprehensive analysis of both spectral and parametric accuracy. The obtained identification results by the parametric error for the first structure indicate that the hybrid model provides the value $\varepsilon_\theta(hybrid) = 0.012$ compared to 0.031 for the neural network and 0.048 for the physical models. For the second structure, these values are $\varepsilon_\theta(hybrid) = 0.013$, 0.027 and 0.041, respectively. This indicates a significant increase in the identifiability of the parameters by the developed model. At the same time, the training time satisfies the ratio $t_{phys} < t_{NN} < t_{hybrid}$. Along with this, the additional computational costs are compensated by the increase in accuracy, stability and reproducibility of the results. Despite the increase in training time, the achieved accuracy and stability make the training algorithm suitable for high-precision spectral digital twins.

Research of model adaptability. To evaluate the adaptive properties of the digital spectral twin, a series of numerical experiments with variable external conditions was conducted. These conditions can be dictated by the variation of layer thicknesses, temperature-induced perturbations of optical constants or linear degradation of films. During the modeling process, the structure parameters changed in time, after which the hybrid model was retrained online using a two-loop algorithm. The dynamics of adaptation was analyzed using the time dependences $\Delta J(t)=\left|J(t)-J^*\right|$ and $\Delta\theta(t)=\left\|\theta(t)-\theta^*\right\|$, where J^* and θ^* correspond to the stationary regime after adaptation. The decrease in these time dependences, after each perturbation, indicates the ability of the model to maintain the correctness of the identification of parameters and, accordingly, restore consistency with the experimental data. Fig. 10 and Fig. 11 show the obtained research results for both synthetic structures.

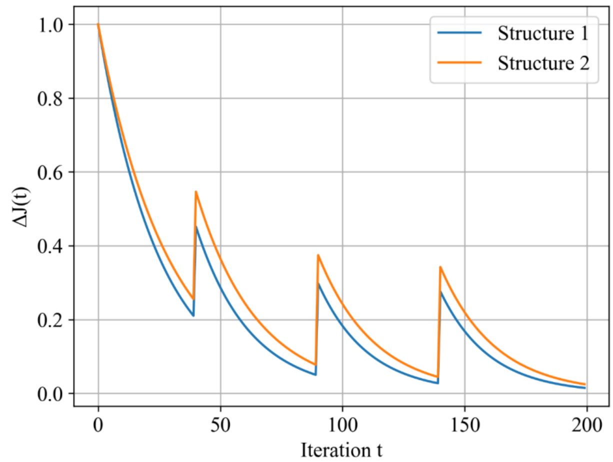

Fig. 10. Dynamics of the residual functional $\Delta J(t)$ in the process of model adaptation for multilayer structures

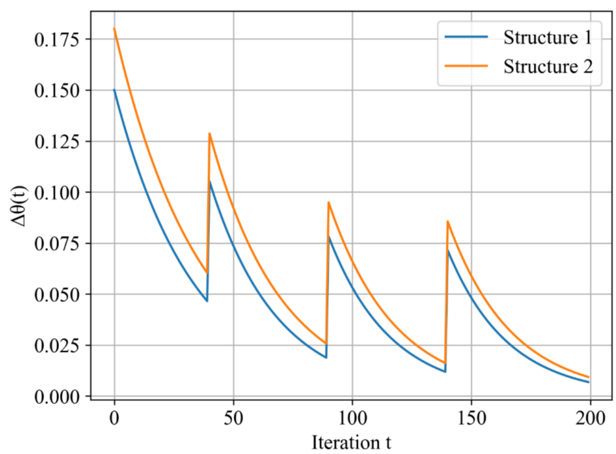

Fig. 11. Dynamics of the parametric error $\Delta\theta(t)$ in the process of model adaptation for multilayer structures

The graphs show sharp increases in the time dependences $\Delta J(t)$, $\Delta\theta(t)$, corresponding to the moments of external disturbances associated with changes in thickness, temperature, and material degradation. Further exponential reduction in errors indicates effective parameter readjustment within the two-loop algorithm. From the figures, it is possible to see that both structures are characterized by stable repetitive adaptation after each disturbance, which additionally confirms the robustness and online adaptability of the developed model. In general, the results obtained confirm the efficiency of the two-loop adaptation mechanism, including under non-stationary conditions.

Research of the dependence of the parameter identification error on the noise level. A numerical experiment was conducted that demonstrates the dependence of the parameter identification error on the noise level, the results of which are shown in Fig. 12.

To implement spectral noise for synthetic spectra, the following formula $\Lambda_{syn}=P(\theta)+\eta$ was chosen. For different noise levels η, the identification error norm $\|\theta^*-\theta\|$ was estimated. The graph shown in Fig. 12 demonstrates a quasi-linear increase in the error with increasing noise. Additionally, the error remains limited, which in turn confirms the identifiability of the parameters. The numerical experiment performed is optimal for formal confirmation of identifiability, since it is based on fully controlled data and does not depend on experimental measurement errors.

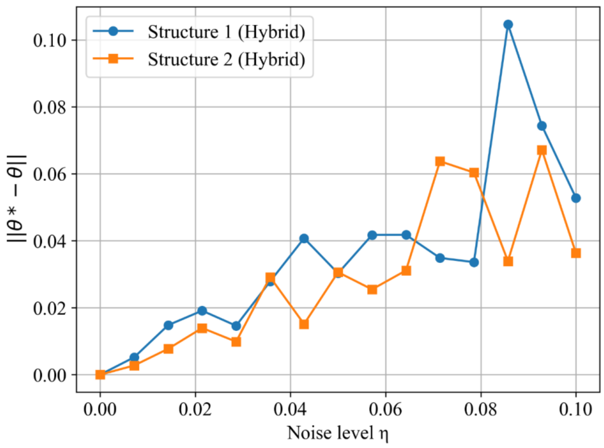

Fig. 12. Parameter identification error depending on the noise level

3.5. Discussion of the results

Unlike classical methods of regularization of inverse problems [4–6], where stabilization parameters are set a priori or determined heuristically, in this research a two-loop mechanism of their coordinated adaptation in the process of training a digital spectral twin is implemented. Unlike neural network methods of spectral approximation [8], as well as physically informed neural networks [9, 10], the developed model, within the framework of information technology, is not limited to the approximation of the solution, but implements a composite operator architecture with an explicit separation of the physical operator, adaptive spectral filter and correction neurooperator. Compared with operator neural network models of the DeepONet type [12], the developed information technology is focused on selective spectral identification and preservation of the physical interpretability of parameters. Its practical advantage is confirmed in the part of numerical verification (Table 2, Fig. 8, 9), where the inequality $RMSE_{hybrid} < RMSE_{NN} < RMSE_{phys}$ is fulfilled, as well as in experimental testing (Fig. 6), which demonstrated the selective localization of the dominant spectral lines of the electrode material against the background of impurity components. The obtained results of dynamic verification additionally confirm the adaptability of the model to changes in parameters over time. The main difference of information technology based on an operator-oriented model is that it combines interpretability and adaptability within a single operator structure. The article formalizes for the first time the integral operator structure of a digital spectral twin with the introduction of a spectral information operator and theoretical conditions of identifiability and convergence, which distinguishes the developed information technology from existing ones, where such aspects were not systematically considered.

The practical significance of the results obtained lies in the possibility of their application for high-precision identification of parameters of multilayer structures, optimization of optical coatings and creation of adaptive digital spectral twins in real time. The developed model is also suitable for tasks of spectral identification of plasma systems and for diagnostics of erosion processes of electrodes. Due to the possibility of online adaptation, it can be used in monitoring and control systems of technological processes, where its continuous coordination with experimental data is necessary.

The features of the obtained results are the development of a holistic operator model of a digital spectral twin, which is built on the basis of the decomposition of the process of forming a spectral response. A two-loop hybrid learning algorithm has been developed, which provides separate but consistent optimization of the physical and neural parameters of the model. An important component is the introduction of the spectral informativeness operator as a separate parameterized block of the model being trained. This block allows formalizing the contribution of informative spectral components to the process of identifying parameters. Theoretical conditions for identifiability, stability and convergence have been developed for the class of hybrid operator models of digital twins, which provides an analytical justification for the correctness of the developed information technology. A variational formulation of the problem of adapting a digital twin is proposed, taking into account physical constraints and regularization mechanisms, which increases the stability of solving incorrect inverse problems.

The uniqueness of the research lies in the fact that the digital spectral twin is considered as a single hybrid operator in functional spaces with an internal adaptation structure, and not as a separate physical or purely neural model. Unlike existing methods and models, the work is not limited to imposing physical constraints on the residual functional, but an architecture is formed in which physical laws and spectral informativeness are the constituent elements of the operator being trained. The balance between physical correctness and the approximation ability of the neural network is ensured by the implemented mechanism of consistent two-loop parameter update. Within the framework of the research of digital twins, the article combines the rigorous mathematical apparatus of operator theory in combination with modern methods of neural network training. The advantages of the work are that the developed model allows ensuring the physical consistency of the results and, at the same time, excludes non-physical solutions that are characteristic of purely neural network models. Due to the implemented decomposition of the parametric synthesis problem, the dimensionality of the optimization is reduced and its conditionality is improved. The implemented two-loop learning mechanism increases the resistance to noise and model perturbations. The developed model architecture has high interpretability, since each of its blocks corresponds to a specific physical process. Additionally, stable convergence of the algorithm is ensured even with limited data volumes. The developed model is scalable and can be adapted to different types of spectroscopic systems.

The limitations of the applicability of the developed information technology include the fact that its effectiveness significantly depends on the correctness of the physical model of the object and the accuracy of parameterization. Its effectiveness also depends on the quality and representativeness of the training sample, which at this stage was formed mainly on the basis of synthetic data, which in turn imposes restrictions on the degree of generalization of the obtained results for the conditions of real technological processes, in particular in cases of significant noise.

The internal shortcomings of the developed model include increased computational complexity compared to classical numerical methods, which is due to the presence of a two-loop optimization procedure and the need for coordinated tuning of physical and neural network parameters. In addition, at the current stage of implementation, the developed model does not fully take into account the complex nonlinear and non-stationary effects of real technological processes, which may limit the accuracy of reproducing the object's behavior.

The research was carried out under martial law in Ukraine. At the same time, it should be noted that the region of its conduct is Transcarpathia, namely the city of Uzhhorod, which is characterized by a relatively more stable security situation compared to most regions of Ukraine. This made it possible to ensure the continuity of the educational process and scientific activity. Of course, air alarms and organizational restrictions took place, but their intensity did not lead to a systematic cessation of research. Despite the nationwide restrictions of the war period, the results obtained in the work confirm the possibility of conducting systematic scientific research in our region, provided that the process is adaptively organized and digital technologies are effectively used. Further research may be aimed at experimental verification of the model in the context of industrial facilities. Its application for multi-physical processes is promising, taking into account thermal, mechanical and chemical factors. It is also advisable to develop adaptive strategies for automatic selection of the neurooperator structure and regularization parameters. Researches of stochastic and Bayesian versions of the digital twin are of considerable interest, including for quantitative assessment of uncertainties. Also, a promising direction is the integration of the model into real-time process control systems and its extension to other types of inverse problems in photonics, materials science and nanotechnology.

4. Conclusions

1. The work developed a hybrid physical-neural operator model of a digital spectral twin with an explicit decomposition into a physical block, a spectral filter and a neurooperator, which allowed to form a holistic mathematical architecture of the model.

2. A two-loop adaptive learning algorithm was constructed, which provides coordinated optimization of physical and neurooperator parameters within a single error functional. Theoretical conditions for stability, convergence and identifiability of the hybrid model were obtained, and the approximation error was estimated, which for synthetic structures does not exceed 0.01, which creates a formal basis for analyzing the correctness of solving inverse spectral problems. The algorithm was implemented programmatically and numerical verification was carried out on two synthetic multilayer structures.

3. Numerical verification of the hybrid model was carried out on synthetic multilayer structures. It is found that for the first structure, $RMSE$ decreases from 0.07 (TMM) to 0.04 (MLP) and to 0.01 in the hybrid model, however, with a simultaneous increase in R from 0.94 to 0.97 and to 0.994. For the second structure, $RMSE$ decreases from 0.06 (TMM) to 0.03 (MLP) and to 0.01 within the hybrid architecture, while R increases from 0.95 to 0.975 and to 0.996. The results clearly confirm the stable advantage of the hybrid model, both in terms of spectral accuracy and consistency of the shape of the reproduced dependencies.

4. The effectiveness of the learning algorithm is assessed and the adaptability of the model is investigated. It is shown that the hybrid architecture provides a stable reduction in error (up to $RMSE \approx 0.1$) and an increase in the consistency of spectral dependencies ($R \approx 0.994$–0.996), which indicates its effectiveness and robustness to variations in input data.

The model was also tested on experimental spectra of high-voltage nanosecond discharge with zinc electrodes. The results confirmed its ability to selectively identify spectral components in complex multiline spectra.

The practical value of the results of the work lies in the possibility of using the developed digital twin model and its training algorithm for highly accurate identification of parameters of multilayer structures, optimization of optical coatings, and construction of adaptive digital twins in real time.

Conflict of interest

The authors declare that they have no conflict of interest regarding this research, be it financial, personal, authorial, or other, which could affect the research and its results presented in this article.

Financing

The research was conducted without financial support.

Data availability

The manuscript has no associated data.

Use of artificial intelligence

The ChatGPT artificial intelligence model (version GPT-5.3, OpenAI) was used in the preparation of the manuscript.

AI tools were used exclusively at the auxiliary stages of manuscript preparation, namely to check the grammar, spelling and punctuation of individual fragments of the text, as well as for preliminary search for literary sources. AI was also used for automated checking of the language design of the text, but without changing its content and for generating lists of potentially relevant scientific sources (last 5 years). All selected literary sources were subsequently precisely checked by the authors. No substantive part of the manuscript (abstract, introduction, methods and models, results and discussion, and conclusions) was created or generated using AI tools.

All of the above results obtained in the manuscript using AI tools were carefully checked by the authors. In particular, language edits were manually checked for compliance with the scientific style, and the used literary sources were checked and edited using scientific databases.

Artificial intelligence tools did not affect the research results, their interpretation and formulated conclusions, and all the main provisions of the manuscript were obtained by the authors independently.

Authors' contributions

Yurii Bilak: Conceptualization, Methodology, Validation, Formal analysis, Investigation, Writing – review and editing, Project administration; ***Antonina Reblian***: Conceptualization, Methodology, Writing – original draft; ***Beata Matyashovska***: Validation, Writing – original draft; ***Emilian Herashchenkov***: Software, Visualization.

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