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Controlled spectral parameter synthesis based on an adaptive informative subset

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ABSTRACT

The **relevance** of the study is due to the increasing complexity of inverse spectroscopy problems arising in materials science, optoelectronics and related fields, as well as the limitations of classical methods of spectral synthesis of parameters, which are based on the use of the full spectrum. This leads to high computational costs, reduced numerical stability and deterioration of the identifiability of parameters in the presence of noise. In this regard, it is relevant to develop methods that provide a controlled reduction in the dimensionality of spectral data without losing the physical correctness and accuracy of parameter synthesis. The **aim** of the work is to develop a method of controlled spectral synthesis of parameters, in which the inverse spectral problem is solved on an adaptively formed informative subset of the spectrum. To achieve the set goal, the following tasks were solved: the concept of spectral informativeness was formalized based on the sensitivity analysis of parameters; a mechanism for adaptive formation of an informative spectral subset was developed; A controlled computational cycle of parameter synthesis using a physically based model was constructed; criteria for stability and stopping the synthesis process were determined. The work applied **methods** of mathematical modeling of spectral characteristics, variational optimization methods, sensitivity analysis, regularization of inverse problems, and principles of controlled computational processes. In the developed method, spectral synthesis of parameters is considered not as a one-time optimization procedure, but as a closed controlled cycle with dynamic adaptation of the spectral region of analysis. The **results** obtained demonstrate that the use of an adaptive informative subset of the spectrum allows to significantly reduce the amount of spectral data while maintaining an admissibly small relative error in parameter estimation. It is shown that in the process of iterative controlled synthesis, weakly informative spectral sections are automatically excluded, for which the sensitivity of the model to parameter variations is low or degenerate, which directly leads to an improvement in the conditionality of the inverse problem. The reduction of spectral redundancy and the concentration of analysis on informative areas ensure the reduction of the influence of noise disturbances on the identification results and the stabilization of the functional minimization process. As a result of numerical testing, the existence of a compromise between the accuracy of parameter synthesis and the volume of spectral information used was confirmed, which within the framework of the developed method is implemented in a controlled, reproducible and without loss of physical interpretability of the results. The method was tested on experimental spectral data of a nanosecond discharge plasma, which confirmed its suitability for the identification of Zn, N₂ and N II concentrations. The practical significance of the results obtained lies in the possibility of increasing the efficiency and stability of inverse spectroscopic calculations in applied information systems.

Keywords: Controlled synthesis; spectral analysis; inverse problems; controlled method; adaptive subset; parameter sensitivity

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INTRODUCTION

Inverse spectroscopy problems play a key role in modern research on materials, optoelectronics, nanophotonics and related fields, as they allow to restore the physical and structural parameters of objects from their spectral characteristics. In most practical cases, such problems are incorrectly posed, sensitive to measurement noise and are characterized by high computational complexity. This necessitates the use of specialized numerical and regularization methods and to ensure the stability and physical correctness of the results. Traditional spectral the

calculations and worsens the convergence of the algorithms synthesis of parameters, as a rule, is formulated as a problem of minimizing the functional of the discrepancy between the model and experimental spectra over the entire available spectral region, which has a number of limitations. The use of the full spectrum leads to excessive computational costs, reduced numerical stability in noise conditions and poor identifiability of individual parameters, the spectral sensitivity of which is localized or insignificant. As a result, part of the spectral information actually does not participate in the synthesis process, but at the same time complicates.

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Recent research in the field of inverse problems, sensitivity analysis and physically based modeling shows that the informativeness of spectral data is uneven along the wavelength and significantly depends on the desired parameters. This opens up the possibility of transitioning from global use of the spectrum to localized analysis of those spectral regions that contain maximum information about the parameters of the object. At the same time, most of the existing methods for selecting spectral ranges are heuristic in nature and are not integrated into the general structure of the synthesis process. In this regard, the development of information technologies is relevant, within which spectral synthesis of parameters is considered not as a one-time optimization procedure, but as a controlled computational process with dynamic adaptation of the spectral region of analysis, stopping criteria and regularization parameters. This allows combining the physical correctness of the model, numerical stability and computational efficiency.

In this paper, a method of controlled spectral synthesis of parameters using an adaptive informative subset of the spectrum is developed. The main idea is to form and dynamically update the spectral domain of analysis based on the assessment of the sensitivity of the parameters, the stability of the synthesis process and the conditionality of the inverse problem. This allows to significantly reduce the dimensionality of the problem without losing the accuracy of parameter recovery and to ensure controlled convergence of the computational process.

Purpose and objectives. The purpose of the work is to develop a method for controlled spectral synthesis of parameters using an adaptive informative subset of spectral data, which allows for effective and stable solution of inverse spectral problems, reducing the amount of calculations without losing the physical correctness of the results.

The objectives of the work are as follows:

1) to theoretically substantiate the concept of controlled spectral synthesis as a closed loop with dynamic selection of the spectral region and stopping criteria;

2) to develop an algorithm for forming an adaptive informative subset of spectral data based on the analysis of the spectral sensitivity of the parameters and the assessment of the conditionality of the inverse problem;

3) to integrate the physical model of the object into the computational cycle to ensure the physical correctness of the synthesis results;

4) to determine the criteria for stability and error control of the synthesized parameters for the controlled cycle;

5) to compare the effectiveness of the developed method with classical synthesis methods through numerical experiments and error analysis.

The paper is structured as follows: Section 2 presents the theoretical foundations of controlled spectral parameter synthesis and formulates the concept of an adaptive informative spectral subset. Section 3 describes the developed architecture of the controlled computational cycle and the corresponding mathematical models and criteria. Section 4 reports the results of numerical experiments and comparative analysis with the classical spectral synthesis methods. The final section summarizes the main conclusions and outlines directions for future research.

RELATED WORKS

Traditional methods for solving inverse problems are based on the minimization of regularized variational functionals and iterative smoothing schemes. The current state of this theory is described in the book [1], which presents in detail the theory of regularization, operator methods and numerical algorithms for ill-posed problems. This theory is widely used to stabilize spectral inversion, but it significantly depends on the choice of the regularization parameter and scales poorly in high-dimensional parameter spaces. In [2], an in-depth interpretation of Tikhonov regularization is developed through the concept of approximate source conditions, which refines the convergence properties, but does not eliminate the sensitivity to noise and the difficulties of discrete implementation in practical spectroscopic problems. An alternative class of traditional methods is iterative regularizers, in particular the Landweber method and its modifications [3], which are characterized by simplicity of implementation, but require empirical selection of the stopping criterion and are characterized by low computational efficiency for problems with a large number of parameters. Separately, modern studies of the Backus–Gilbert method [4] should be highlighted, which include its probabilistic and Bayesian generalizations, and extend its classical variation to multiparameter inverse problems, while providing the possibility of integrating a priori information. In general, traditional methods are limited by high computational cost, sensitivity to noise and regularization parameters, as well as insufficient physical interpretability of solutions, which

necessitates the transition to adaptive and physically informed methods of spectral synthesis.

Adaptive and reduced spectral methods are aimed at overcoming the limitations of classical regularizations by reducing the dimensionality of the search space. In [5], [6], the Adaptive Spectral Inversion (ASI) method was developed, in which the inverse problem is solved in an adaptive spectral subspace with a dynamically changing basis of eigenfunctions, which allows implementing implicit regularization without introducing penalty terms and significantly reducing computational costs. At the same time, such methods are closely related to a specific direct operator and require specialized tuning, which limits their versatility. Bayesian adaptive methods, in particular inversion using Polynomial Chaos Kriging [7], implement active selection of informative sections of the parameter space and provide effective approximation of posterior distributions with a limited number of calls to the direct model. However, without explicit integration of the physical model, such methods may lose physical interpretability and complicate stability analysis. Additionally, recent works demonstrate the development of adaptive and modified classical numerical methods to improve the stability and accuracy of spectral inversion. In [8], a method for solving inverse spectral problems with incomplete data was developed, which allows for correct reconstruction of spectral characteristics even with limited information. A similar idea of adaptive optimization was implemented through a modification of the classical Levenberg–Marquardt algorithm [9], which provides increased convergence and stability when inverting spectra with noise and complex spectral structures. It is also worth mentioning the method developed in [10], which effectively selects representative subsets, but is focused on classification problems and requires physical adaptation for spectral inversion, which limits its universality. Adaptive selection of subsets from LUT databases [11] allows for reducing computational costs and increasing the accuracy of inversion, but depends on the density and representativeness of the table, which also limits its capabilities without physical regularization. This emphasizes the need to combine LUT methods with physical models and adaptive selection of informative subsets. In general, adaptive spectral methods reduce the computational complexity of inverse problems, but are characterized by limited universality, dependence on the specific formulation, and increased methodological complexity.

Further development of adaptive methods is represented by hybrid methods that combine physical models with machine learning methods for solving inverse spectral problems. In [12], a physically oriented model based on a regularized recurrent inference network was developed, where physical constraints are integrated directly into the learning and inversion process, which provides increased noise resistance and reduced need for training data. A similar in ideology, but less physically rigorous strategy is presented in [13], where the reconstruction of spectral functions is carried out through automatic differentiation, and regularization is implemented implicitly through the architecture of the neural network; at the same time, the lack of explicit physical priors may limit the interpretability of the solution.

Significant progress in physically informed machine learning is associated with the development of adaptive PINN-like architectures. In [14], [15], [16], [17], various adaptation mechanisms have been developed, from guided tuning of kernels and hyperparameters to spectral and residual architectures aimed at overcoming spectral bias, loss balancing problems, and unstable derivative optimization. They demonstrate increased accuracy and efficiency in problems with sharp gradients or complex spectral structures, but are accompanied by an increase in architectural and algorithmic complexity. The application of physically informed neural networks to inverse problems in materials science and multiphysics systems is considered in [18], where the possibility of reliable inversion of anisotropic parameters and physically significant characteristics is shown. In [19], a hybrid model of inverse spectral analysis of multilayer structures was developed, combining pre-trained deep neural networks with classical iterative algorithms, providing increased accuracy, noise resistance, and reduced iterations, which confirms the effectiveness of integrating physical models and machine learning. The importance of choosing informative regions of the spectrum was investigated in [20], where the example of plasma physics shows which spectral components critically affect the accuracy of parameter determination. The results obtained emphasize the need to integrate knowledge about spectral relevance into computational algorithms and adaptive methods. General trends in spectral methods are summarized in [21], which considers a wide range of methods for solving nonlinear problems, their strengths and weaknesses, and the possibilities of integration with modern ML- and physically-informed methods. The paper [22]

demonstrates the modern development of methods for spectral decomposition of hyperspectral data, where, along with classical geometric, statistical and sparsity-oriented methods, modern deep learning and hybrid methods for analyzing spectral mixtures are also considered. A vivid example of adaptive reduction of the spectral space is the paper [23], where the effectiveness of representative learning by selecting relevant bands is demonstrated. However, the method does not contain an explicit physical interpretation of spectral parameters, which may complicate its application in spectroscopy, where the physical consistency of the solution is critical. Modern parameter-efficient methods, in particular [24], demonstrate significant capabilities for fine-tuning models using only an information-significant subset of parameters, which reduces computational costs and the risk of overtraining, but requires a reliable assessment of the information significance of the selected parameters to preserve the physical consistency of the model.

In general, ML- and physics-informed methods and models open up new opportunities for solving complex inverse spectral problems, but their application is limited by the dependence on the quality of training data, the risk of overfitting and spectral biases of neural networks, which makes the development of hybrid adaptive methods with explicit consideration of the physical structure of the problem relevant. Similar variations of increasing the efficiency of neural network models by optimizing training procedures and controlling the dynamics of gradient descent are considered in [25], where the possibility of accelerating and stabilizing the training of neural networks in applied information systems is demonstrated. The practical application of the ML model to the analysis of spectral characteristics is also demonstrated in [26], where a combined machine learning model for interpreting spectral data of gas mixtures is developed, which confirms the effectiveness of integrating machine learning algorithms with physically based spectral analysis models.

Thus, the review confirms the trend towards adaptive dimensionality reduction and selection of informative subsets as a means of improving the efficiency of inversion problems. Their strengths are the reduction of computational costs and improvement of data representativeness. At the same time, the existing limitations are the lack of explicit physical interpretability and dependence on the specificity of the data. This is consistent with the position of this article that for spectral synthesis it is necessary to integrate adaptive algorithms with

physically based models and mechanisms for selecting informative components.

RESEARCH METHODOLOGY

Research hypothesis. Assumptions and simplifications adopted. The research hypothesis is that the developed method of controlled spectral synthesis of parameters, which uses an adaptive informative subset of spectral data, allows to achieve comparable or higher accuracy of parameter recovery compared to classical synthesis over the full spectrum, while simultaneously reducing the amount of calculations and ensuring controlled stability of the synthesis process.

Certain assumptions and simplifications are adopted in the work. The spectrum of the object is considered as a linear superposition of modal components, which allows estimating the sensitivity of parameters locally within the selected subset of the spectrum. The structure of the object and the basic physical properties of materials are considered known and do not change during the synthesis of parameters. Spectral measurements contain additive noise with known statistical characteristics, which does not depend on the parameters. A limited finite number of parameters is synthesized, which provides the possibility of using normalized error metrics. Changes in the spectral subset Λ_l occur gradually, according to the sensitivity assessment, to avoid sharp jumps in errors and ensure the stability of the controlled cycle.

Conceptual formulation of the problem. Let a physical object be described by a vector of parameters

$$\vec{p} = (p_1, p_2, \dots, p_N), \quad (1)$$

and its spectral characteristic is formed by a direct physical model

$$S_{\text{mod}}(\lambda, \vec{p}): \Lambda \rightarrow R, \quad (2)$$

where $\lambda \in \Lambda = [\lambda_{\min}, \lambda_{\max}]$ is a full spectral region.

Experimentally measured spectrum:

$$S_{\text{exp}}(\lambda) = S_{\text{true}}(\lambda) + \varepsilon(\lambda), \quad (3)$$

where $\varepsilon(\lambda)$ is an additive measurement noise [27].

Classical inverse problem (constraints). Traditionally, spectral synthesis of parameters is formulated as the minimization of a functional over the entire spectral domain:

$$\vec{p}^* = \arg \min_p \int_{\Lambda} |S_{\text{mod}}(\lambda, \vec{p}) - S_{\text{exp}}(\lambda)|^2 d\lambda, \quad (4)$$

where \vec{p}^* is a parameter estimation. Despite its formal universality, this problem is characterized by a high dimensionality of the parameter space and, as a result, significant computational costs. In addition, integration over the entire spectral region leads to excessive calculations in areas that are poorly informative about the desired parameters, reduces the robustness of the problem to experimental noise, and complicates the identification of individual parameters whose contribution to the spectrum is local or correlated with others.

In such a formulation, the structure of the inverse problem is considered fixed throughout the synthesis process, which makes it impossible to adapt it to local spectral properties and the current state of parameter identification.

Adaptive informative subset of the spectrum.

To overcome these limitations, a mechanism for quantifying the local informativeness of the spectrum is introduced, which is subsequently used as a control signal.

Definition of information content. To assess the impact of each parameter on the spectrum, a *spectral information content function* is introduced:

$$I(\lambda, \vec{p}) = \sum_{i=1}^N \omega_i \left| \frac{\partial S_{\text{mod}}(\lambda, \vec{p})}{\partial p_i} \right|, \quad (5)$$

where ω_i are the parameter weights, and the derivatives describe the sensitivity of the spectrum to parameter changes. If $\partial S_{\text{mod}}/\partial p_i \approx 0$, the parameter p_i is practically not identified in this region of the spectrum [28], [29].

Formation of the informative region. Expansion or narrowing of the informative region is carried out based on changes in the functional and local spectral informativeness:

$$\Lambda_I^{(k+1)} = \begin{cases} \Lambda_I^{(k)} \cup \Delta\Lambda, & \text{if } \Phi^{(k)} - \Phi^{(k-1)} < \varepsilon_\Phi \\ \Lambda_I^{(k+1)} \setminus \Delta\Lambda, & \text{if } k(J_{\Lambda_I}^{(k)}) > k_{\text{max}} \end{cases}. \quad (6)$$

The informative spectral subset is defined as the set of wavelengths for which the informativeness measure exceeds a given adaptive threshold:

$$\Lambda_I = \{\lambda \in \Lambda \mid I(\lambda, \vec{p}) \geq \tau\}, \quad (7)$$

where τ is an adaptive information threshold.

In this formulation, the informative region Λ_I is a proper subset of the full spectral region Λ , and its dimension is significantly smaller compared to Λ . This allows us to focus computational resources only on the most informative parts of the spectrum, eliminating the need to process the full spectral

range and increasing the efficiency and robustness of the algorithm. Thus, the use of the full spectral range is not necessary for effective parameter identification.

Controlled spectral synthesis of parameters.

The control rules C determine how and when the inverse problem statement itself changes in the process of spectral synthesis of parameters. The formation and adaptation of the informative spectral region within the controlled synthesis is carried out in accordance with definitions (5)-(7) and is considered as one of the controlled mechanisms for restructuring the inverse problem. The basic state variables are the current estimate of the parameters of the physical model at the k -th iteration $\vec{p}^{(k)}$, $\Lambda_I^{(k)}$ – the current informative spectral region formed on the basis of the analysis of the sensitivity of the spectrum to the parameters, the value of the residual functional $\Phi^{(k)}$ and the numerical characteristics of the conditionality of the inverse problem. The control rules analyze the dynamics of these quantities and form decisions regarding the further restructuring of the synthesis process.

Controlled computational cycle. Formally, controlled spectral synthesis is described as a controlled computational system given by a tuple

$$T = \langle \vec{p}^{(k)}, \Lambda_I^{(k)}, M, C \rangle, \quad (8)$$

where M is a parameterized physical model of spectral characteristic formation, C is a set of governing rules that determine the mechanisms for adapting the synthesis process, which is introduced by the authors.

Within the framework of this algorithm, each iteration of the synthesis process not only specifies the values of the parameters $\vec{p}^{(k)}$, but is also accompanied by an analysis of the informativeness of the spectral data, an assessment of the stability of the inverse problem and, if necessary, a correction of the spectral domain of analysis. Thus, spectral synthesis acquires the properties of a controlled process, in which not only the sought solution changes, but also the structure of the problem itself.

The control rules C implement the decision logic for expanding or narrowing the informative spectral region, changing the spectral discretization resolution, correcting the regularization parameters, and switching between different optimization modes. This allows for a consistent combination of accuracy, computational efficiency, and numerical stability of the synthesis process.

The control rules C are given as a set of decision operators that act on the state of the computational process at the k -th iteration.

$$S^{(k)} = (\vec{p}^{(k)}, \Lambda_I^{(k)}, \Phi^{(k)}, J_{\Lambda_I}^{(k)}), \quad (9)$$

where $\Phi^{(k)}$ is the value of the functional; \vec{J}_{Λ_I} is the sensitivity matrix (Jacobian) calculated on the current informative spectral subset $\Lambda_I^{(k)}$.

Rules for forming an informative region. The above mechanism for forming an informative spectral subset within the framework of controlled synthesis is implemented in the form of formal control rules that operate at each iteration of the process and are implemented according to formulas (6-7).

The adaptation regularization rules are adjusted based on the assessment of the conditionality of the tasks:

$$\alpha^{(k+1)} = \alpha^{(k)} \cdot \begin{cases} \gamma_+, k(J_{\Lambda_I}^{(k)}) > k_{\max} \\ \gamma_-, k(J_{\Lambda_I}^{(k)}) < k_{\min} \end{cases}, \quad (10)$$

$\gamma_+ > 1, \gamma_- < 1.$

As the number of conditions increases, regularization is strengthened to stabilize the solution, while as the conditions improve the value of α decrease, which increases the accuracy of parameter synthesis. This allows stabilizing the synthesis in areas of poor parameter identifiability.

The rules for selecting the optimization mode are determined by the value of the gradient of the functional:

$$M^{(k)} = \begin{cases} \text{global search, } \|\nabla_p \Phi^{(k)}\| > \delta_1 \\ \text{local refinement, } \delta_2 < \|\nabla_p \Phi^{(k)}\| \leq \delta_1 \\ \text{stabilization, } \|\nabla_p \Phi^{(k)}\| \leq \delta_2 \end{cases}. \quad (11)$$

The developed mechanism for controlled formation and adaptation of an informative spectral subset, as well as a system of governing rules for making decisions regarding the structure of the computational process is the author's development and has no direct analogues in known works on classical spectral synthesis of parameters.

Controlled synthesis functional. In a controlled computational cycle, the local residual functional is minimized, defined not on the full spectral domain, but only on its informative subset:

$$\Phi^{(k)}(\vec{p}) = \int_{\Lambda_I^{(k)}} |S_{\text{mod}}(\lambda, \vec{p}) - S_{\text{exp}}(\lambda)|^2 d\lambda + \alpha R(\vec{p}), \quad (12)$$

where S_{mod} is a spectrum obtained from the physical model M ; S_{exp} is an experimentally measured spectrum, R is a regularization functional reflecting a priori constraints on the model parameters [30], α is an adaptive regularization coefficient.

The main feature of this computational cycle is that the functional $\Phi^{(k)}(\vec{p})$ changes during the synthesis process together with the informative spectral region $\Lambda_I^{(k)}$. This means that at each iteration a different local inverse problem is solved, optimally matched to the current state of the parameters and the properties of the spectrum. The adaptive coefficient α provides a balance between the accuracy of the approximation of the experimental data and the stability of the restored parameters. Its value is adjusted based on the analysis of the convergence of the process, the sensitivity of the spectrum to the parameters and the conditionality of the corresponding sensitivity matrix. Due to this, the controlled spectral synthesis of the parameters allows avoiding re-adaptation to measurement noise, automatically detecting regions with low informativeness and providing physically correct and numerically stable solutions to the inverse spectral problem.

Stopping criteria as a control element. Synthesis stops not only based on error, but on a set of criteria:

$$\begin{cases} \|\vec{p}^{(k+1)} - \vec{p}^{(k)}\| < \varepsilon_p \\ \|\Lambda_I^{(k+1)} - \Lambda_I^{(k)}\| < \varepsilon_\Lambda, \\ k(\vec{J}_{\Lambda_I}) < k_{\max} \end{cases}, \quad (13)$$

where k is a the conditionality number [31]. This set of criteria is the author's addition to the classical formulation of the Dirichlet problem and allows us to control the stability and accuracy of parameter synthesis in the process of a controlled cycle. As a result, we have a stop for the stability of the process, not just the result.

RESULTS AND DISCUSSION

Algorithm and architecture. Fig. 1 shows the developed architecture of controlled spectral synthesis of parameters with a closed feedback loop, in which the parameters of the physical model and the informative spectral region are adaptively updated until stability criteria are achieved.

Algorithm of controlled spectral synthesis of parameters. Let us dwell in detail on the main steps of the developed algorithm.

Step 1. Initialization. Initial estimates of the object parameters $\bar{p}^{(0)}$, the initial spectral region $\Lambda_I^{(0)} \subset \Lambda$, as well as the initial control settings are given: regularization coefficient $\alpha^{(0)}$, spectral resolution $\Delta\lambda^{(0)}$ and stopping criteria.

Step 2. Physical modeling. Based on the current parameters $\bar{p}^{(k)}$ within the informative region $\Lambda_I^{(k)}$, the model spectrum

$$S^{mod}(\lambda, \bar{p}^{(k)}), \lambda \in \Lambda_I^{(k)}$$

is calculated using the physical model M .

Step 3. Controlled spectral synthesis of parameters. The inverse problem is solved by minimizing the local functional (12), resulting in an updated parameter estimate $\bar{p}^{(k+1)}$.

Step 4. Analysis of convergence and informativeness (control module). Based on the iteration results, the convergence of the parameters $\|\bar{p}^{(k+1)} - \bar{p}^{(k)}\|$, the sensitivity of the spectrum to the parameters, and the conditionality of the inverse problem in the current domain $\Lambda_I^{(k)}$ are estimated. The control module generates control rules for the next iteration.

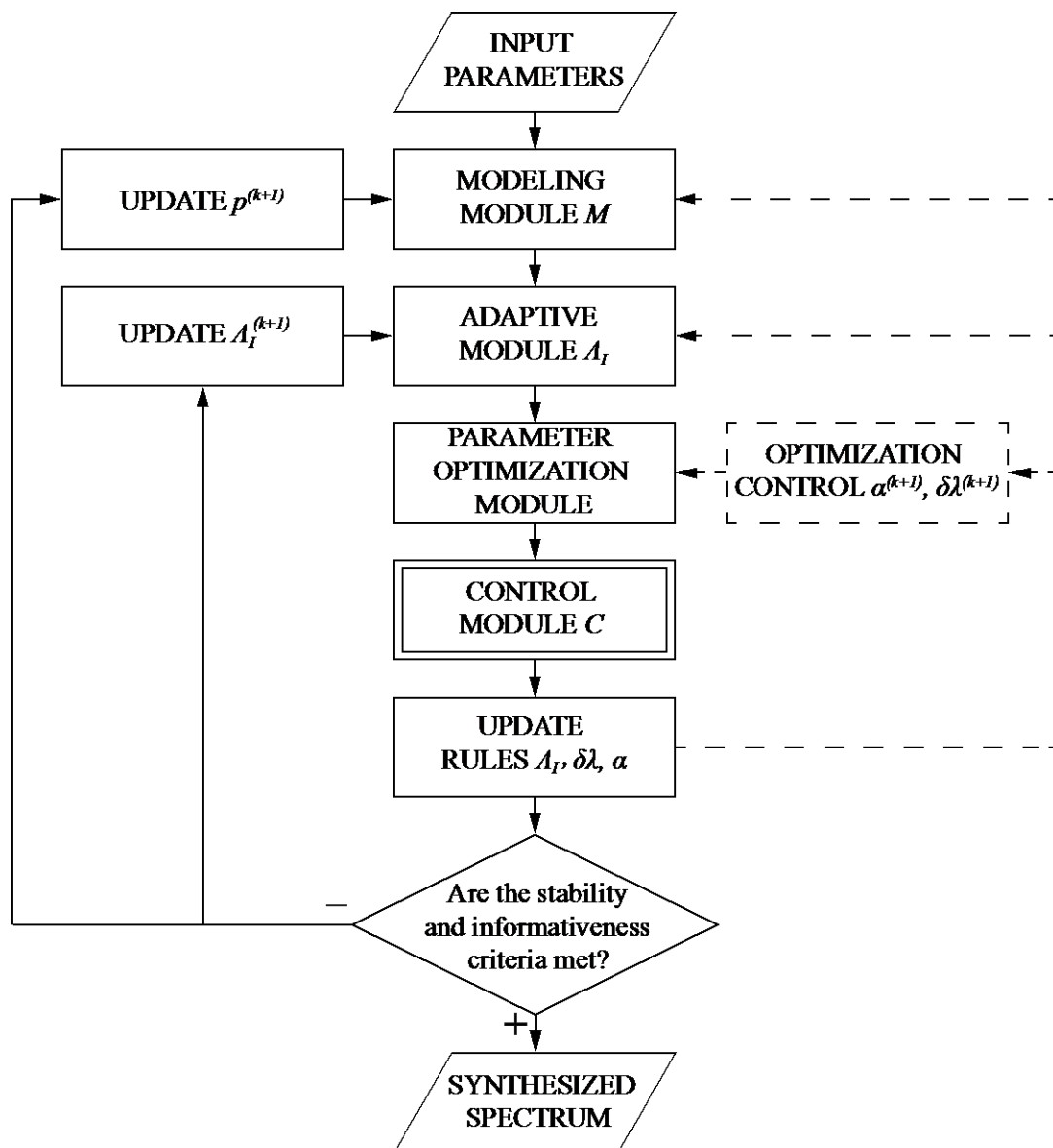


Fig. 1. Architecture of controlled spectral synthesis of parameters with closed feedback loop

Source: compiled by the authors

Step 5. Adaptation of the computational strategy. According to the governing rules, the informative spectral region $\Lambda_I^{(k)} \rightarrow \Lambda_I^{(k+1)}$ is adjusted, the spectral resolution $\Delta\lambda^{(k+1)}$ is changed, and the regularization coefficient $\alpha^{(k+1)}$ is adapted.

Step 6. Checking the stopping criteria. The stability and informativeness conditions (13) are checked. If the conditions are met, the algorithm ends with the final estimates \bar{p}^* . If not, then the transition to the next iteration $k \leftarrow k+1$ is made.

Thus, parameter synthesis is implemented as a closed-loop controlled loop in which the adaptation of the spectral domain and computational parameters is based on convergence, sensitivity, and conditionality analysis, rather than following a fixed or heuristic scheme.

Numerical testing and accuracy analysis. To demonstrate the performance of the developed method of controlled spectral synthesis of parameters, synthetic spectral data were used, formed according to a generalized physically interpreted model in the form of a sum of two Gaussian components that simulate individual spectral contributions without being tied to specific chemical elements or materials. This allows us to investigate the properties of controlled spectral synthesis in a universal setting, independent of the specifics of a particular object.

The full spectral range Λ covers the region of 400–800 nm, which contains both informative and weakly sensitive regions. To analyze the effectiveness of adaptive spectral reduction, several informative subsets of Λ_I of different widths were considered, concentrated in regions of increased spectral sensitivity to model parameters. This choice allows us to investigate the influence of the size and localization of Λ_I on the accuracy of synthesis and computational efficiency.

Regarding the analysis of spectral approximations, Fig. 2 is constructed, which shows a comparison of the experimental (noise) spectrum with the results of classical parameter synthesis performed using the full spectral range Λ . We see that involving the entire spectrum does not guarantee optimal agreement with experimental data, since weakly informative regions of the spectrum negatively affect the stability of the inverse problem.

Fig. 3 illustrates the results of the developed controlled parameter synthesis for several variants of informative subsets Λ_I . Despite the significant reduction in the spectral range, the model spectra demonstrate high agreement with the experimental data precisely in the informative regions. This

confirms the feasibility of the transition from the full spectrum to an adaptively formed subset.

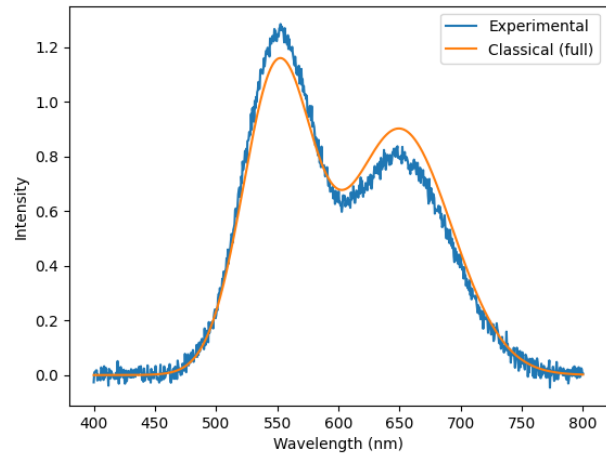


Fig. 2. Classical synthesis (full spectrum)

Source: compiled by the authors

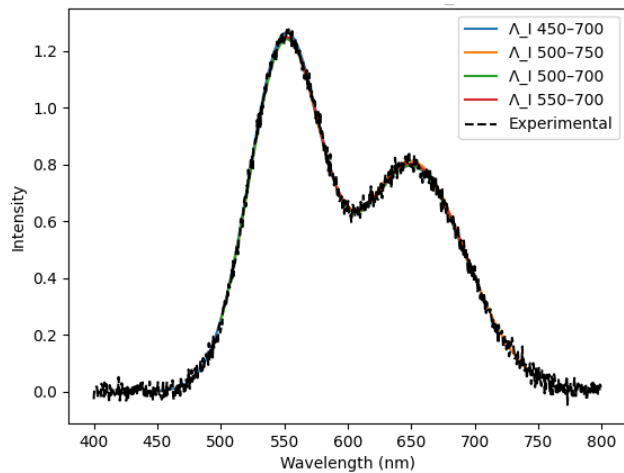


Fig. 3. Controlled synthesis for different Λ_I

Source: compiled by the authors

Fig. 4 shows the relative error of parameter estimation for different variants of Λ_I . The obtained results indicate that reducing the spectral range does not lead to a significant deterioration in the accuracy of the synthesis. On the contrary, for some informative subsets, more stable and more reproducible parameter estimation is observed, which is explained by the improvement of the conditionality of the inverse problem.

Fig. 5 shows the ratio $|\Lambda_I|/|\Lambda|$, which characterizes the fraction of the used spectrum relative to the full range. We see that in the considered scenarios only 30–60 % of the spectral points are used, which directly reduces the computational costs and the amount of processed data.

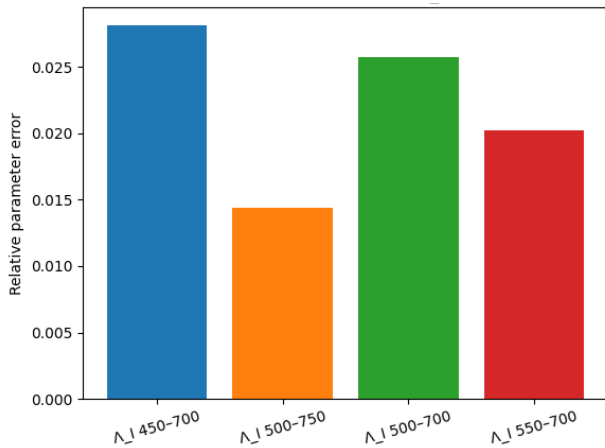


Fig. 4. Parameter estimation error
Source: compiled by the authors

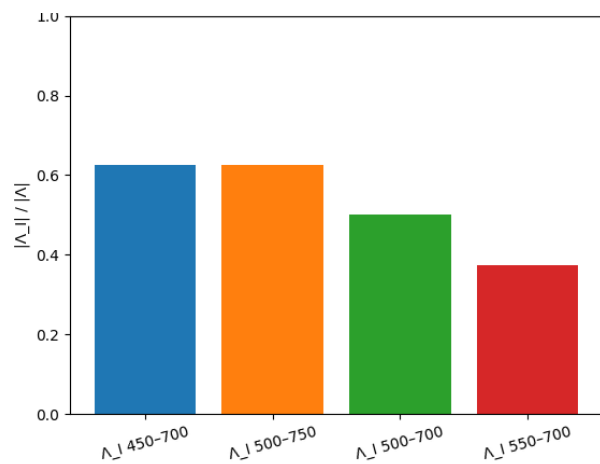


Fig. 5. Spectral reduction efficiency
Source: compiled by the authors

It should be noted that spectral dependences in this article are used not as the ultimate goal of analysis, but as an information carrier for solving the problem of model parameter synthesis. The obtained spectra serve as a means of verifying the correctness of the identified parameters, while the main criterion for the effectiveness of the developed method is the accuracy of the estimation of the object parameters.

Fig. 6 shows the results obtained to illustrate the influence of the size of the informative spectral region on the accuracy of parameter recovery and to quantitatively confirm the effectiveness of guided spectral synthesis under the conditions of stepwise reduction of spectral information. Four informative spectral regions $\Lambda_I^1 \rightarrow \Lambda_I^2 \rightarrow \Lambda_I^3 \rightarrow \Lambda_I^4$ are displayed on the X axis.

These spectral regions $\Lambda_I^{(k)}$ are selected as follows:

- $\Lambda_I^1 = [450, 750]$ nm, $|\Lambda_I^{(1)}| = 300$ nm – wide region, almost classical synthesis;

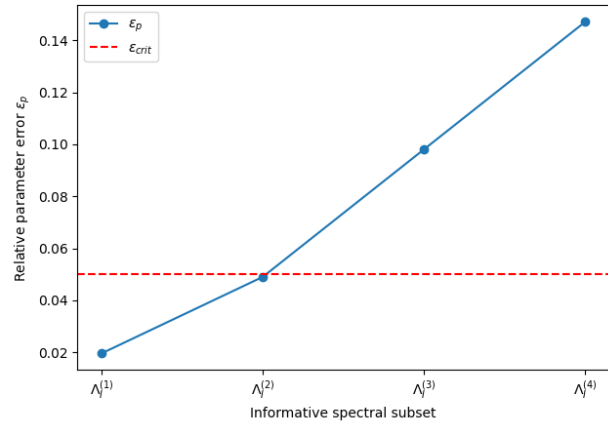


Fig. 6. Four informative spectral regions to demonstrate controlled parameter synthesis
Source: compiled by the authors

- $\Lambda_I^2 = [500, 700]$ nm, $|\Lambda_I^{(2)}| = 200$ nm – middle region, weakly informative edges of the spectrum are eliminated;

- $\Lambda_I^3 = [550, 650]$ nm, $|\Lambda_I^{(3)}| = 100$ nm – narrow region, zone of maximum parametric sensitivity;

- $\Lambda_I^4 = [580, 620]$ nm, $|\Lambda_I^{(4)}| = 40$ nm – minimum area, critical minimum information.

The ordering is performed by the width of the spectral area as follows $|\Lambda_I^1| > |\Lambda_I^2| > |\Lambda_I^3| > |\Lambda_I^4|$ (300 > 200 > 100 > 40). That is, there is more spectral information on the left, and less on the right.

The Y axis shows the relative error of parameter estimation:

$$\epsilon_p = \frac{\|\vec{p}^* - \vec{p}_{ref}\|}{\|\vec{p}_{ref}\|}$$

The increase in the relative error ϵ_p with a decrease in the size of the informative spectral region Λ_I is expected and is due to a decrease in the amount of available information. At the same time, the results demonstrate that the developed controlled spectral synthesis provides a stably acceptable accuracy of parameter recovery even with a significant spectral reduction, which indicates the information efficiency of the method. We see that there is a compromise between the accuracy of parameter synthesis and the amount of spectral information used. Even with a significant reduction in the spectrum, when $|\Lambda_I| \ll |\Lambda|$, the relative error ϵ_p remains acceptably small. The developed method operates in a controlled manner under conditions of

incomplete information, and does not “fall” chaotically.

The horizontal red line corresponds to the permissible error ε_{crit} , which is defined as the maximum permissible deviation of the synthesized parameters from their reference values. The value $\varepsilon_{crit}=0.05$ (5 %) was chosen as representative for the demonstration problem, which meets the typical requirements for synthesis accuracy in spectral modeling of such systems. It shows that with a relative error of less than 5 %, the parameters are considered to be adequately restored, which allows us to clearly compare the efficiency of controlled synthesis for different informative regions Λ_I . As we can see, for the first two, wider spectral regions $\varepsilon_p < \varepsilon_{crit}$, which indicates a high accuracy of parameter synthesis. For narrower regions, the error increases and exceeds ε_{crit} , demonstrating the expected compromise between the amount of spectral information and the accuracy of parameter restoration. The obtained result confirms the effectiveness of the developed method, i.e. even with partial spectral reduction, the accuracy remains acceptable for the most informative ranges.

Therefore, the presented results clearly demonstrate that the adaptive informative subset of the spectrum Λ_I allows to significantly reduce the amount of spectral data without loss of informativeness, the accuracy of parameter synthesis remains stable or even improves due to conditionality control, and the developed architecture implements not just optimization, but a controlled method of spectral parameter synthesis, where spectral reduction is a systemic element of the algorithm.

Comparison with classical synthesis. Table 1 presents a comparative analysis of the developed parameter synthesis method with classical synthesis. Classical synthesis is a one-time optimization of the functional, without assessing the sensitivity or stability of the parameters, while the developed method implements a closed controlled loop with

dynamic adaptation of the parameters and the spectral domain. The stopping criteria in controlled synthesis include not only minimizing the functional, but also checking stability and sensitivity, which increases noise resistance and ensures the physical correctness of the restored parameters through the integration of the physical model into the loop. The flexibility of the system is also significantly higher, due to the fact that the method allows you to automatically change the resolution of the spectrum and focus on informative areas, which is not available to classical synthesis.

Spectral identification of gas mixtures. In experimental works [32], [33], [34], a study 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, to demonstrate the capabilities of the developed method, the task of spectral identification of plasma components of an overvoltage nanosecond discharge between zinc electrodes in a nitrogen atmosphere was chosen [32]. In the experiment, Zn I / Zn II lines (zinc vapor), the N₂ Second Positive System system, N II lines and a weak background and measurement noise are observed. The task is to determine the concentration contributions of the components $C=\{Zn, N_2, N^+\}$ from the measured emission spectrum.

A model spectrum in the range of 200–600 nm was formed based on informative lines (subset Λ_I). Zn: 206.20, 213.85, 330.25, 334.50, 472.21 nm; N₂: 315.93, 337.13, 357.69 nm; N II: 399.49, 462.13, 500.52, 567.60 nm were selected. The peak amplitudes were taken proportional to the relative intensities given in the experimental article. The lines were modeled by Gaussian profiles ($\sigma=0.25$ nm).

Table 1. Comparison with classical synthesis

Characteristics	Classical synthesis	Controlled adaptive synthesis
Spectrum usage	Full spectrum	Adaptive informative subset
Process type	One-shot optimization	Closed controlled loop
Stopping criteria	Functional minimization only	Minimization + stability + sensitivity
Computational cost	High	Less due to spectrum reduction
Noise resistance	Medium	Higher, due to sensitivity analysis
Physical correctness	Partially	Preserved, due to model integration into the loop
Flexibility	Low	High, dynamic control of parameters and spectrum area

Source: compiled by the authors

Fig. 7 shows the simulated experimental spectrum of plasma emission from an overvoltage nanosecond discharge between zinc electrodes in a nitrogen atmosphere. The blue signal displays the full measured spectrum including all registered lines, background component and detection noise, which corresponds to the real experimental situation. On this background, only those spectral components that were used in the concentration identification task are highlighted in color.

The yellow color reproduces the contribution of atomic and ionized zinc (Zn), which corresponds to a fraction of 0.25 and characterizes the electrode material. The green color indicates molecular nitrogen N_2 (Second Positive System) with a dominant fraction of 0.65, which determines the main volume of the plasma. The red color shows the lines of ionized nitrogen N II with a fraction of 0.10, which reflect the degree of ionization of the discharge medium. Other weak lines (O II, Ar II, N I) remain in the background spectrum and are not involved in the parametric identification procedure. These values correspond to the physical picture of the process, namely, nitrogen dominates, and zinc vapors from the electrodes and an ionized component are present. Such visualization demonstrates the localization of the informative part of the spectrum within the general measured signal, which justifies the use of the adaptive informative subset Λ_I for a stable assessment of the concentrations of the plasma mixture components.

Additionally, a comparison of minimization functionals was performed to demonstrate the impact of the full spectral range and the adaptive informative subset Λ_I on the stability of Zn

concentration estimation. Here, the problem of Zn concentration estimation with other components fixed is modeled.

The graph in Fig. 8 shows that the functional constructed over the entire spectrum has additional local minimum regions due to the influence of noise and background. The functional limited to the subset Λ_I has a more pronounced global minimum near the true concentration value, which demonstrates increased stability and reduced sensitivity to parasitic effects.

Thus, the experimental testing showed that the informative part of the spectrum is localized in narrow areas associated with the characteristic lines Zn, N_2 and N II, while the full spectral range contains a significant background and noise contribution. The use of the adaptive subset Λ_I ensures a reduction in the dimensionality of the problem and the formation of a more pronounced global minimum of the functional, which increases the stability of concentration identification. The results obtained confirm the feasibility of using the developed method for problems of spectral analysis of gas mixtures in plasma environments.

To demonstrate the advantages of the developed method, the problem of the dependence of the error in the identification of spectral parameters on the noise level was considered. The study was conducted on the basis of inverse analysis of the emission spectrum using two methods, namely classical inversion (on the full spectrum) and the developed method (on an adaptively formed subset of informative spectral lines). The obtained results of the identification of the Zn concentration are shown in Fig. 9.

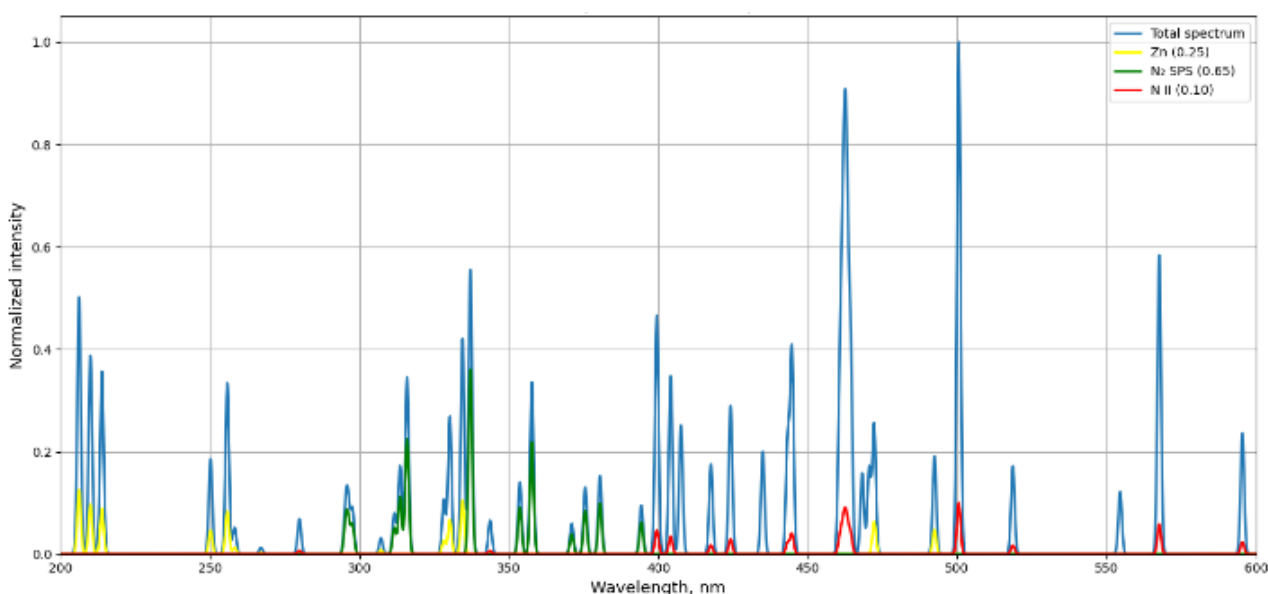


Fig. 7. Simulated emission spectrum with component contributions

Source: compiled by the authors

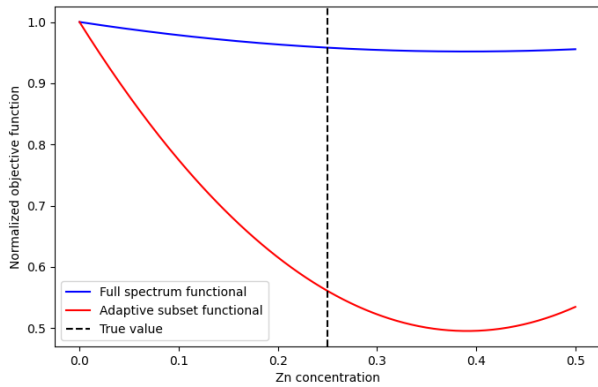


Fig. 8. Comparison of minimization functionals
Source: compiled by the authors

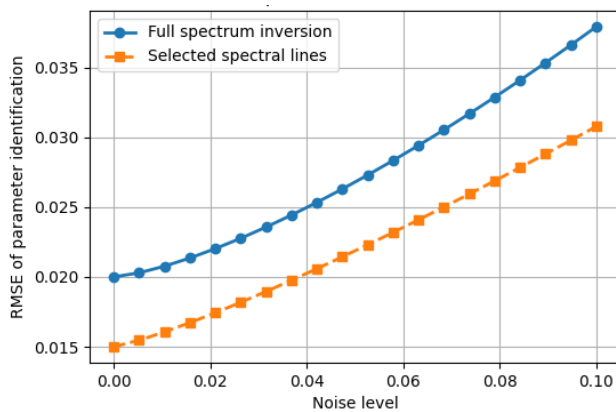


Fig. 9. Dependence of Zn concentration identification error on noise level for the full spectrum and adaptive subset
Source: compiled by the authors

Analysis of the graph shows that with increasing noise level from 0 to 20 %, the error in identifying Zn concentration for both methods increases, however, the method based on the adaptive subset of informative lines demonstrates consistently lower RMSE values. At low noise, the error is ≈ 0.002 - 0.003 and decreases to ≈ 0.010 at 20% noise, while for the full spectrum the error increases from ≈ 0.005 to ≈ 0.018 - 0.020 . This indicates increased resistance of the method to noise distortions and better localization of the global minimum of the optimization functional.

Discussion. The obtained results of numerical testing confirm the feasibility of transitioning from the classical full-spectrum formulation of the inverse problem to the controlled spectral synthesis of parameters, formally described by equations (1)-(4). As shown in the article, minimization of the residual functional over the entire spectral domain leads to excessive participation of weakly informative regions of the spectrum, which negatively affects the conditionality of the problem and increases sensitivity to noise. Similar limitations of classical

methods are also noted in works [1], [2], [3], [4], where a fixed spectral region is used without taking into account parametric sensitivity.

The mechanism for forming an informative spectral subset developed in the work, mathematically substantiated in formulas (5)-(8) and illustrated in Fig. 2 and Fig. 3, allows focusing the synthesis process on those regions of the spectrum that carry the maximum information about the sought parameters. Unlike the heuristic methods for selecting spectral intervals considered in [5], [6], [7], [8], in this work, spectrum reduction is carried out based on sensitivity analysis and properties of the inverse problem, which ensures the formalized and reproducible nature of the procedure.

An important result is the improvement of the conditionality of the parameter identification process, which follows from the analysis given in formulas (9)-(11). As shown in the results of numerical experiments, a decrease in the number of spectral variables is accompanied by a decrease in the correlation between the parameters and stabilization of the minimization process. In traditional spectral synthesis methods described in [2], [6], [9], such a problem often leads to the non-identification of some parameters or the appearance of multiple solutions.

The reduction in the noise effect recorded in the work is explained by the fact that the adaptively formed subset of the spectrum does not include areas with a low signal-to-noise ratio and weak dependence on the parameters, which is consistent with analytical considerations. Unlike full-spectrum methods [3], [4], [13], where noise components directly affect the functionality, in the developed method their effect is significantly limited at the stage of controlling the synthesis process.

It should also be noted that the analysis of the relative error of parameter estimation (Fig. 4) shows that the reduction of the spectral domain does not lead to a proportional deterioration in accuracy. For informative subsets of medium and large width, the relative error of parameters remains below the permissible level $\varepsilon_{crit}=0.05$, which indicates the preservation of parametric informativeness even with significant spectral reduction. The improvement of stability for individual Λ_i is explained by the decrease in the conditionality number of the sensitivity matrix, which is consistent with the stopping criteria (see formula (13)). The results shown in Fig. 5 quantitatively confirm the effectiveness of spectral reduction: in the considered scenarios, only 30-60 % of spectral points from the

full range of Λ are used. This directly reduces the computational costs and makes the synthesis process more suitable for integration into real-time or quasi-real-time information systems. Thus, resource savings are achieved not at the expense of accuracy loss, but due to the controlled selection of informative data. Analysis of four informative spectral regions of different widths (Fig. 6) clearly demonstrates the compromise between the amount of spectral information and the accuracy of parameter recovery. With excessive narrowing of Λ_i , a controlled increase in error is observed, but even in this case the algorithm remains stable and does not enter the incorrect identification mode. This fundamentally distinguishes the developed technology from classical methods [7], [13], [14], [15], where spectrum reduction usually leads to uncontrolled degradation of the solution.

The results of testing on experimental data demonstrate that the use of an adaptive informative subset of spectral lines provides a clearer localization of the global minimum of the optimization functional compared to the analysis of the full spectral range (Fig. 8). When the noise level increases to 20 %, the error in identifying the Zn concentration for the developed method is about 0.010, while for the classical one, on the full spectrum, it increases almost twice (Fig. 9), which indicates the increased resistance of the method to noise distortions. The localization of informative spectral sections within the characteristic lines of Zn, N₂ and N II (Fig. 7) allows reducing the influence of background components and overlapping of spectral lines characteristic of the plasma of overvoltage nanosecond discharges. Thus, the adaptive formation of the subset Λ_i actually implements a physically justified reduction in the dimension of the inversion problem, which increases the stability and accuracy of estimating the concentrations of the components of the plasma mixture.

The developed method is most effective for spectral identification problems of multicomponent systems with partially overlapping lines, the presence of a background component and measurement noise – in particular for emission spectra of plasma, gas discharges, laser-induced plasma, as well as for optical spectra with localized informative maxima. The greatest effect of using an adaptive subset is achieved in cases where the spectrum contains a limited number of physically interpreted informative sections, while the rest of the range forms a noise or weakly informative

component, which generates parasitic local minima of the functional. Under such conditions, the reduction of the minimization space increases the identifiability of parameters and the stability of the solution. On the other hand, the advantages of the method are leveled for smooth nonlinear spectra (broadband absorption curves without clear localization of maxima), for high-signal measurements with insignificant noise, and also in cases where the entire spectral range is uniformly informative. In such problems, using the full functional does not lead to the appearance of parasitic minima, and adaptive reduction does not provide a significant gain.

In general, the analysis of the results confirms that the developed architecture of the guided spectral synthesis implements not just parameter optimization, but a guided computational process in which spectral reduction, regularization adaptation and stopping criteria work in concert to ensure stability, accuracy and computational efficiency.

The uniqueness of the work lies in the treatment of spectral synthesis of parameters as a guided method with adaptive reduction of spectral data, where the process of parameter identification is guided on the basis of sensitivity analysis, conditionality and stability of the inverse problem. Unlike existing methods, the adaptation of the spectral domain is integrated directly into a closed computational loop and has a formalized, rather than heuristic, nature.

The limitations and disadvantages of the developed method include the fact that the efficiency of controlled spectral synthesis significantly depends on the adequacy of the selected physical model and the correctness of the estimation of the spectral sensitivity of the parameters; in the case of model errors or an inaccurately specified object structure, the advantages of adaptive spectrum reduction may decrease. The developed method is focused on problems with a relatively limited number of parameters, for which sensitivity and conditionality analysis is computationally acceptable; with a significant increase in the dimensionality of the parameter space, control costs may increase. The use of adaptive information thresholds and control criteria requires preliminary tuning, which may affect the universality of the method for different classes of spectral problems. In addition, the method requires the calculation of derivatives or their numerical approximations, which may be limiting for extremely complex models.

The scientific novelty of the work lies in the development of a new paradigm for solving inverse spectral problems, within which spectral synthesis of parameters is implemented as a controlled method, and not as a one-time optimization procedure. Unlike classical methods, the developed architecture provides for dynamic adaptation of the spectral domain of analysis, the structure of the computational process and stopping criteria in accordance with the current state of the problem. For the first time, adaptive spectral reduction is implemented based on the sensitivity analysis of parameters, the conditionality of the inverse problem and the control of the stability of the synthesis, which allows to significantly reduce the dimensionality of the problem without losing the physical correctness of the results. The obtained results formalize spectral synthesis of parameters as an intelligently controlled computational process that combines physically based modeling and adaptive processing of spectral data.

Further research should be directed at expanding the method of controlled spectral synthesis of parameters to more complex physical models, in particular multiparameter and nonlinear spectrum-forming systems with a large number of interconnected parameters. It is promising to generalize the mechanisms for forming an informative spectral subset for cases of multidimensional spectral data, as well as for problems with spatial-spectral or temporal-spectral dependence. Of particular interest is the integration with machine learning methods for automated prediction of informative spectral regions and adaptation of control rules based on accumulated data. This will allow us to move from fixed control criteria to self-consistent intelligent strategies of spectral synthesis. A practical direction of development is the implementation of the method in the form of a software package or service for use in applied information systems of spectroscopic analysis, in particular in conditions of limited computing resources or real time. It is also promising to study the impact of various types of noise and measurement errors on the stability of controlled synthesis and formalize adaptive strategies for compensating for such effects. In general, further development of the developed method opens up opportunities for creating intelligent controlled systems for solving inverse spectral problems, capable of automatically balancing between accuracy, stability and

computational efficiency depending on the application conditions.

CONCLUSIONS

Theoretical analysis of the developed method allowed substantiating a number of fundamental advantages of controlled spectral synthesis of parameters. It is shown that the use of an adaptive informative subset of the spectrum leads to a reduction in the dimensionality of the inverse problem without loss of parametric informativeness. By excluding weakly informative spectral regions, the conditionality of the synthesis problem is improved and the sensitivity of the results to measurement noise is reduced. Spectral sensitivity analysis allows detecting and excluding from the synthesis process parameters that are not identified in the current spectral region, which increases the stability and physical interpretability of the solution. The combination of these effects provides a significant saving of computational resources and increases the efficiency of the numerical implementation of the inverse spectral problem.

The paper develops and tests a method of controlled spectral synthesis of parameters, in which the inverse spectral problem is solved on an adaptively formed informative subset of the spectrum. The developed method implements a controlled closed computational cycle with dynamic adaptation of the spectral region of analysis and synthesis parameters.

Within the framework of numerical testing, a comparison of classical spectral synthesis and controlled synthesis was performed for different informative regions, ordered by decreasing their width. It is shown that the transition from the full spectrum to adaptive spectral subsets allows to significantly reducing the number of used spectral points by several times. At the same time, for wide and medium informative regions, the relative error of parameter synthesis remains lower than the specified permissible value $\varepsilon_{crit}=0.05$, which indicates the preservation of high accuracy of parametric identification. The obtained graphical results demonstrate that even with a significant reduction of the spectral region, controlled synthesis provides a close reproduction of the experimental spectrum and a stable estimation of parameters. At the same time, for excessively narrow informative regions, a controlled increase in the relative error of the parameters was recorded, which confirms the existence of a compromise between the accuracy of the synthesis and the amount of spectral information.

It is important that within the framework of this method this compromise is not implemented chaotically, but predictably and controlled.

Testing on experimental spectra showed that the developed method provides correct and stable identification of plasma gas mixture components in the presence of background and noise. Quantitative comparison with the classical optimization method over the full spectrum showed that the use of the adaptive subset AI allows reducing the parameter identification error in the presence of noise and

reducing the sensitivity of the solution to uninformative spectral regions.

Thus, the testing results confirm the hypothesis of the study about the possibility of achieving high accuracy of parameter synthesis with a significantly smaller amount of spectral data. The developed method demonstrates increased computational efficiency and stability compared to classical synthesis, which makes it promising for use in information systems of spectral analysis and solving inverse problems.

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Метод керованого спектрального синтезу параметрів із використанням адаптивної інформативної підмножини

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АНОТАЦІЯ

Актуальність дослідження зумовлена зростаючою складністю обернених задач спектроскопії, що виникають у матеріалознавстві, оптоелектроніці та суміжних галузях, а також обмеженнями класичних методів спектрального синтезу параметрів, які базуються на використанні повного спектра. Це призводить до високих обчислювальних витрат, зниження числової стійкості та погіршення ідентифікованості параметрів у присутності шуму. У зв'язку з цим актуальним є розробка методів, що забезпечують кероване зменшення розмірності спектральних даних без втрати фізичної коректності та точності синтезу параметрів. **Метою** роботи є розробка методу керованого спектрального синтезу параметрів, у якому обернена спектральна задача розв'язується на адаптивно сформованій інформативній підмножині спектра. Для досягнення поставленої мети розв'язано такі завдання: формалізовано поняття спектральної інформативності на основі аналізу чутливості параметрів; розроблено механізм адаптивного формування інформативної спектральної підмножини; побудовано керований обчислювальний цикл синтезу параметрів із використанням фізично-обґрунтованої моделі; визначено критерії стабільності та зупинки процесу синтезу. У роботі застосовано **методи** математичного моделювання спектральних характеристик, варіаційні методи оптимізації, аналіз чутливості, регуляризацію обернених задач та принципи керованих обчислювальних процесів. У розробленому методі, спектральний синтез параметрів розглядається не як одноразова оптимізаційна процедура, а як замкнений керований цикл із динамічною адаптацією спектральної області аналізу. Отримані **результати** демонструють, що використання адаптивної інформативної підмножини спектра дозволяє істотно зменшити обсяг спектральних даних при збереженні допустимо малій відносній похибці оцінки параметрів. Показано, що в процесі ітераційного керованого синтезу відбувається автоматичне виключення слабкоінформативних спектральних ділянок, для яких чутливість моделі до варіацій параметрів є низькою або виродженою, що безпосередньо приводить до покращення обумовленості оберненої задачі. Зменшення спектральної надлишковості та концентрація аналізу на інформативних ділянках забезпечують зниження впливу

шумових збурень на результати ідентифікації та стабілізацію процесу мінімізації функціоналу. У результаті чисельної апробації підтверджено існування компромісу між точністю синтезу параметрів і обсягом використаної спектральної інформації, який у межах розробленого методу реалізується керовано, відтворювано та без втрати фізичної інтерпретованості результатів. Метод апробовано на експериментальних спектральних даних плазми наносекундного розряду, що підтвердило його придатність для ідентифікації концентрацій Zn, N₂ та N II. Практичне значення отриманих результатів полягає у можливості підвищення ефективності та стійкості обернених спектроскопічних обчислень у прикладних інформаційних системах.

Ключові слова: керований синтез; спектральний аналіз; обернені задачі; керований метод; адаптивна підмножина; чутливість параметрів

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