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TECHNOLOGY FOR MODELING PHYSICOCHEMICAL PROCESSES IN THE PLASMA OF OVERVOLTAGE NANOSECOND GAS DISCHARGE FOR THE SYNTHESIS OF NANOSTRUCTURED THIN FILMS AND ITS SOFTWARE IMPLEMENTATION

Context. In this work, for the first time, a technology has been developed based on an integrated physical-mathematical model of the emission spectrum of plasma from an overvoltage nanosecond gas discharge, which is used for the synthesis of nanostructured thin films. Universal software has been developed for modeling plasma parameters and its spectrum, providing interactivity and flexibility for adaptation to various experimental conditions. Visualization of results has been implemented to enhance data analysis and interpretation. The developed software is an effective tool for scientific research and practical applications in plasma physics and materials science.

Objective. To develop a technology based on an integrated model and software for analyzing physicochemical processes in the plasma of an overvoltage nanosecond gas discharge for describing the dynamics of plasma parameters, modeling the plasma emission spectrum, optimizing the conditions for the synthesis of nanostructured thin films, and creating a tool for predicting plasma parameters.

Method. In the article, a combined theoretical-experimental method is used, which includes key aspects such as mathematical modeling for the implementation of physical and spectral models to describe the main processes in plasma, such as gas ionization, recombination, formation of runaway electrons, electrode erosion, and the formation of clusters of nanostructured films; the use of Boltzmann equations for calculating the distribution of particles over energy levels; calculation of the plasma emission spectrum taking into account temperature, Doppler line broadening, and plasma parameters; representation of spectral lines as Gaussian profiles to describe their width and intensity. The model is implemented based on numerical methods for solving differential equations using the Python programming language for modeling physical processes and visualizing results.

Results. The developed technology, the constructed spectra, the numerical modeling conducted, and the developed software confirm the effectiveness of the developed technology based on mathematical modeling for analyzing plasma processes and spectral characteristics. This opens up new possibilities for optimizing plasma technologies and creating innovative materials.

Conclusions. The technology for calculating plasma parameters and emission spectra for the experiment has been tested. Special attention has been paid to modeling spectral lines for key elements such as nitrogen (N), oxygen (O), and tungsten (W), using Gaussian functions to reproduce the widths of the spectral lines. The model has been adapted to predict plasma characteristics under conditions of variable discharge parameters, such as electric field intensity, pressure, and temperature. This allows for the optimization of film synthesis processes and the creation of new materials with improved properties. The proposed approach has practical applications in sensing, optoelectronics, photovoltaics, and other advanced technologies. In the future, a promising direction is the improvement of the technology and, accordingly, the software product by creating an interface for convenient control of model parameters, which will allow the use of the program without deep programming knowledge; integration of the program with cloud computing platforms for modeling complex systems with high performance; and the application of machine learning algorithms for automatic optimization of discharge parameters and result prediction.

Keywords: mathematical modeling; analysis and optimization; plasma emission spectrum; overvoltage nanosecond gas discharge; materials science

БІЛАК ЮРІЙ, ШУАЇБОВ ОЛЕКСАНДР, БУЧУК РОМАН, РОЛЬ МАР'ЯНА
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ТЕХНОЛОГІЯ МОДЕЛЮВАННЯ ФІЗИКО-ХІМІЧНИХ ПРОЦЕСІВ У ПЛАЗМІ ПЕРЕНАПРУЖЕНОГО НАНОСЕКУНДНОГО ГАЗОРОЗРЯДУ ДЛЯ СИНТЕЗУ НАНОСТРУКТУРОВАНИХ ТОНКИХ ПЛІВОК ТА ЇЇ ПРОГРАМНА РЕАЛІЗАЦІЯ

Актуальність. У роботі вперше розроблено технологію, що базується на інтегрованій фізико-математичній моделі спектру випромінювання плазми перенапруженого наносекундного газорозряду, який використовується для синтезу

наноструктурованих тонких плівок. Розроблено універсальне програмне забезпечення для моделювання параметрів плазми та її спектру, яке забезпечує інтерактивність та гнучкість для адаптації під різні експериментальні умови. Реалізовано візуалізацію результатів для покращення аналізу та інтерпретації даних. Розроблене ПЗ є ефективним інструментом для наукових досліджень та практичного застосування у фізиці плазми й матеріалознавстві.

Мета. Розробити технологію на базі інтегрованої моделі та програмне забезпечення для аналізу фізико-хімічних процесів у плазмі перенапруженого наносекундного газорозряду для опису динаміки плазмових параметрів, моделювання спектра випромінювання плазми, оптимізації умов синтезу наноструктурованих тонких плівок, створення інструменту для прогнозування параметрів плазми.

Метод. У статті використано комбінований теоретико-експериментальний метод, який включає такі ключові аспекти як математичне моделювання для реалізації фізичної та спектральної моделей для опису основних процесів у плазмі, таких як іонізація газу, рекомбінація, формування електронів-втікачів, ерозія електродів, і утворення кластерів наноструктурованих плівок; використання рівнянь Больцмана для розрахунку розподілу частинок за енергетичними рівнями; розрахунок спектра випромінювання плазми з урахуванням температури, доплерівського розширення ліній і параметрів плазми; представлення спектральних ліній як гаусівських профілів для опису їх ширини та інтенсивності. Реалізовано модель на основі чисельних методів для розв'язання диференціальних рівнянь з використанням мови програмування Python для моделювання фізичних процесів та візуалізації результатів.

Результати. Розроблена технологія, побудовані спектри, проведене чисельне моделювання та розроблене ПЗ підтверджують ефективність розробленої технології на основі математичного моделювання для аналізу плазмових процесів і спектральних характеристик, що відкриває нові можливості для оптимізації плазмових технологій і створення інноваційних матеріалів.

Висновки. Проведено апробацію технології для розрахунку параметрів плазми та спектру випромінювання для експерименту. Особливу увагу приділено моделюванню спектральних ліній для ключових елементів, таких як азот (N), кисень (O) та вольфрам (W), з використанням гаусових функцій для відтворення ширини спектральних ліній. Модель адаптована для прогнозування характеристик плазми в умовах змінних параметрів розряду, таких як напруженість електричного поля, тиск і температура. Це дозволяє оптимізувати процеси синтезу плівок і створювати нові матеріали з покращеними характеристиками. Запропонований підхід має практичне застосування в сенсориці, оптоелектроніці, фотовольтаїці та інших передових технологіях. У майбутньому перспективним напрямом є вдосконалення технології та, відповідно, програмного продукту засобами створення інтерфейсу для зручного керування параметрами моделі, що дозволить використовувати програму без глибоких знань програмування; інтеграція програми з платформами хмарних обчислень для моделювання складних систем із високою продуктивністю та застосування алгоритмів машинного навчання для автоматичної оптимізації параметрів розряду та прогнозування результатів.

Ключові слова: математичне моделювання; аналіз та оптимізація; спектр випромінювання плазми; перенапружений наносекундний газорозряд; матеріалознавство

Introduction

Thin films play a key role in many modern technologies such as optics, electronics, photovoltaics, biomedicine, and sensors. The development of methods for forming high-quality films with specified properties is critically important for creating new materials and devices. Plasma deposition methods provide unique conditions for material synthesis, such as high temperatures, ionization of atoms and molecules, and the ability to control the composition and structure of materials at the nanoscale. This makes plasma an indispensable tool for obtaining films with complex chemical and physical properties [1].

Plasma deposition methods allow achieving high energy efficiency and provide precise control over the thickness, composition, and structure of films. This is important and relevant for the mass production of devices such as solar cells, OLED displays, or thin-film transistors. The use of plasma enables the creation of nanostructured films with unique properties, such as increased conductivity, optical transparency, or catalytic activity. This opens up new prospects in the creation of functional materials for energy, medicine, and ecology.

Plasma methods can be adapted to work with a wide range of materials, including metals, oxides, nitrides, and polymers. Many of them are environmentally friendly, which aligns with modern requirements for sustainable development. Research in plasma physics expands knowledge about fundamental processes in materials and plasma environments. This contributes to the development of new methods for obtaining films with improved characteristics, which has significant scientific and practical potential and dictates the relevance of the research. Thus, the study of plasma processes is important and relevant for enhancing film deposition technologies and their use in advanced fields of science and technology [2-4].

The aim of the work was to develop a technology based on a theoretical physical-mathematical model and corresponding software for analyzing physicochemical processes in the plasma of an overvoltage nanosecond gas discharge, taking into account its parameters and spectral characteristics to optimize the synthesis of nanostructured thin films. The model should provide analysis of the dynamics of processes in the plasma, model the plasma emission spectrum, and optimize discharge conditions to enhance the quality of the synthesized nanostructured thin films.

Review of the literature

Numerical modeling of plasma processes, in particular, overvoltage nanosecond discharges, is an important direction of modern plasma physics, since these phenomena are widely used in technologies related to plasma chemistry, materials processing, and medicine. Let us consider works that present numerous approaches to plasma modeling, which differ both in complexity and in applicability to various physical conditions. One of the most common approaches is the use of kinetic models, in particular, the solution of the Boltzmann equation to describe the electron distribution function. In [5], kinetic methods demonstrate high accuracy for describing non-equilibrium processes in plasma. The Monte Carlo method described in [6] is effective for modeling electron collisions with molecules and atoms, especially under low pressure conditions. However, kinetic models have significant computational complexity, which limits their application for large scales. PIC is one of the leading methods for plasma modeling, which allows taking into account both microscopic particle dynamics and

macroscopic fields. Works [5, 7] emphasize the versatility of this method, which can be used to describe non-stationary processes, such as the formation of streamers or the development of discharges. In particular, PIC is successfully used to model nanosecond discharges under atmospheric pressure conditions [8]. Despite this, the method requires significant computational resources and is sensitive to initial conditions. Hydrodynamic models are also widely used in the literature to describe plasma as a continuous medium. Works [9, 10] show that such models are effective for quickly estimating plasma parameters in cases where microscopic effects can be neglected. They are successfully used to describe high-pressure discharges and dense plasma, but do not take into account the dynamics of individual particles. Thermodynamic models assume local thermodynamic equilibrium of the plasma and are used under high pressure and temperature conditions. Works [11, 12] show that such approaches allow to simplify modeling, but are unsuitable for non-equilibrium conditions, such as nanosecond discharges. As for combined approaches, the combination of kinetic and hydrodynamic models is reflected in modern studies [13, 14]. These approaches provide a compromise between accuracy and speed of calculations, allowing to describe in detail the interaction of electrons, ions and neutral particles. The disadvantage is the complexity of integrating different models, which can affect the stability and accuracy of the results. In work [15] experimental data on the parameters of nanosecond discharges in air mixtures are presented, which allow to validate numerical models. Such studies demonstrate the agreement between experimental and numerical results, in particular for electron density, drift velocity and electric fields. In work [16] elementary processes of interaction of charged particles in an electron beam with a current of about 1 A are investigated. The results of numerical modeling by the one-dimensional Particle-In-Cell method of such processes as the expansion of the electron gas, the temperature equalization of two subsystems of the electron gas, and the natural oscillations of the model electron-positron and electron-proton gases are presented. Within the framework of the method, the free electron gas expands due to the electrostatic repulsion between electrons at a constant total energy. The model of the free electron gas, which is represented by model particles in the form of infinite plates, is also solved analytically. In [17], a full cycle of experimental and theoretical studies and mathematical modeling of plasma processes in a negative corona under ambient pressure of nitrogen-oxygen and argon-oxygen gas mixtures was carried out. The influence of the geometric and electrical parameters of oxygen on the current pulsation was studied. The corona current was numerically simulated using differential continuity equations for charge flows, supplemented by the Poisson equation for the electric field in quasi-two-dimensional space. Physical mechanisms of a complex corona current pulse as a precursor, as well as a pulse step and high-frequency current pulsations are defined. In [18] it was shown that the most acceptable physical model for describing plasma oscillations during plasmon generation is the cold plasma model, where we use standard fluid equations to obtain an expression for plasma oscillations. Particular attention in the work is paid to the use of the Particle-In-Cell method, with the help of which the modeling and visualization of plasma oscillations was carried out using the MathCad program code.

Experimental studies were also conducted in a number of scientific works that require further modeling and processing of the obtained experimental data. In the articles [19–23], various aspects of overvoltage nanosecond discharges and their application for the synthesis of thin films and nanostructures were investigated. In [19], the spectral characteristics of the plasma between zinc electrodes were studied and the synthesis of nanostructured films of zinc, zinc oxide and zinc nitride was realized. In [20], the plasma between aluminum and chalcopyrite electrodes was investigated, which allowed the synthesis of CuAlInSe2 films and the determination of key plasma parameters. In [21], the effect of laser radiation on the formation of structured films from an aqueous solution of copper sulfate was analyzed. In [22], the features of the discharge in nitrogen between silver sulfide (Ag2S) electrodes, which can be a source of UV radiation and microstructured films, are described. In [23], a method for the synthesis of WO3 films in a gas-vapor mixture “Air–W” without vacuum technology was proposed. For these works, numerical modeling of processes is relevant due to the complexity and resource intensity of experiments. The literature review indicates significant progress in numerical modeling of plasma, especially using kinetic methods and the PIC method. These approaches are the most effective for describing non-equilibrium processes characteristic of nanosecond discharges. However, the high computational complexity remains a challenge, which stimulates the development of combined models that combine the advantages of different approaches. Further research can be aimed at improving the efficiency of calculations and integrating experimental data to improve numerical models.

Materials and methods

Let focus on the development of a technology based on a theoretical model to explain the above-described experiments and its software implementation. The model encompasses the following physical processes: modeling gas ionization, electrode erosion, cluster formation, and plasma emission spectrum, and is based on the use of numerical methods for solving differential equations. The emission spectrum model is built on Gaussian profiles to describe the widths of spectral lines.

As the programming environment, the *Python* programming language was chosen, which has several advantages for scientific computations, thanks to libraries like *numpy* (for numerical calculations), *scipy* (for solving differential equations), matplotlib (for visualizing results), and *sympy* (for analytical calculations).

During the development of the program code, the following modular structure was designed:

1. Gas Ionization Module contains the implementation of the equation for the change in the concentration of charged particles:

$$\frac{dn_e}{dt} = \alpha n_e v_e - \beta n_e^2 \quad (1)$$

The input parameters are *E,p,T*. The implemented function is used to calculate the concentration n_e as a function of time.

2. Runaway Electrons Module contains the electron energy equation:

$$\frac{dW_e}{dt} = eE - v_e W_e \quad (2)$$

Input parameters: E, v_e. The result of the module is a function to calculate W_e as a function of time.

3. Electrode Erosion Module is implemented using the evaporation formula:

$$\dot{m}_W = \frac{P_A}{\sqrt{2\pi m_W k_B T_W}} \quad (3)$$

Input parameters: T_W, P_A . The result of the module is a function to calculate the evaporation rate.

4. Cluster Formation Module contains the nucleation equation:

$$\frac{dN_k}{dt} = J_k - \beta_k N_k^2 \quad (4)$$

Module input parameters J_k ,β_k. The result is a function to calculate the cluster concentration N_k depending on time.

Below is a fragment of the code listing of the developed integrated software application that implements all the above-described stages of the model (ionization, formation of runaway electrons, electrode erosion, and cluster formation).

```
# Ionization
alpha = 1e-7  # Ionization coefficient, m³/s
beta = 1e-13  # Recombination coefficient, m³/s
v_e = 1e6  # Electron velocity, m/s
n0 = 1e16  # Initial electron concentration, m^-3

# Runaway Electrons
E = 1e7  # Electric field strength, V/m
nu_e = 1e12  # Electron collision frequency, Hz

# Erosion
P_A = 1e3  # Saturated vapor pressure of tungsten, Pa
T_W = 3000  # Electrode surface temperature, K

# Cluster Nucleation
J_k = 1e10  # Cluster nucleation rate, m^-3/s
beta_k = 1e-12  # Probability of cluster coalescence, m³/s
N_k0 = 1e12  # Initial cluster concentration, m^-3

# Time scale
t_span = (0, 1e-6)  # Time in seconds
t_eval = np.linspace(t_span[0], t_span[1], 1000)

# Modules
# Gas Ionization Module
def electron_concentration(t, n_e):
    return alpha * n_e * v_e - beta * n_e**2

# Runaway Electrons Module
def runaway_electrons(t, W_e):
    return e * E - nu_e * W_e

# Electrode Erosion Module
def tungsten_erosion(t, m_W_rate):
    return P_A / np.sqrt(2 * np.pi * m_W * k_B * T_W)

# Cluster Formation Module
def cluster_formation(t, N_k):
    return J_k - beta_k * N_k**2

# Integration of Modules
# Gas Ionization
sol_ion = solve_ivp(electron_concentration, t_span, [n0], t_eval=t_eval)
```

```
# Runaway Electrons
sol_runaway = solve_ivp(runaway_electrons, t_span, [0], t_eval=t_eval)

# Erosion
m_W_rate = tungsten_erosion(0, None)  # Константна швидкість еродування

# Cluster Formation
sol_clusters = solve_ivp(cluster_formation, t_span, [N_k0], t_eval=t_eval)
```

The program operates as follows. To account for gas ionization, the change in electron concentration over time is calculated; for runaway electrons, the kinetic energy of electrons in the electric field is computed; electrode erosion is calculated through the evaporation rate of the electrode material (in our example, tungsten); for cluster formation, a nucleation model is developed that estimates the concentration of clusters (tungsten oxide) [23].

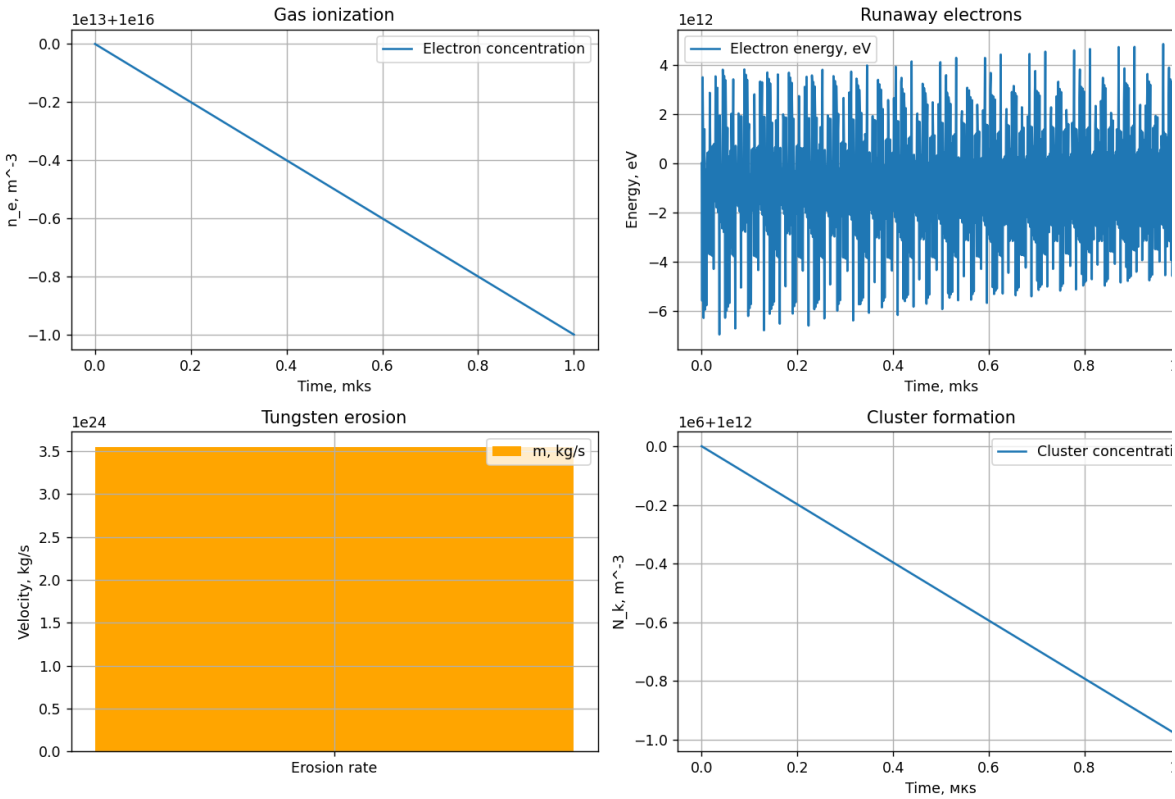

Fig.1. Program Output

To adapt the model to specific tasks, the parameters *E, T_W, and P_A* should be changed, in order to simulate different experimental conditions. Clearly, the model can be improved by adding new modules to account for other physical effects, for example, such as plasma interaction with the substrate, and so on.

Mathematical Model of the Emission Spectrum. The next step was the development of a theoretical model for the plasma emission spectrum in the aforementioned experiments. Different theories can be used for spectrum modeling. Let's focus in more detail on the main ones.

Electron Beam Theory. Emission in plasma occurs due to electron impacts on atoms and molecules. These impacts lead to the excitation of atoms and molecules, and subsequently, their emission occurs. The spectrum will be characterized by several spectral lines, where each line corresponds to a transition between energy levels.

Boltzmann Model for Level Population. The distribution of particles in plasma can be described using the Boltzmann distribution, which allows estimating the probability of occupation of energy levels depending on the temperature:

$$N_i = N_0 \frac{g_i}{Z(T)} exp\left(-\frac{E_i}{k_B T_e}\right), \quad (5)$$

where N_i — the number of particles at level i, g_i — the statistical weight of the energy level, E_i — the energy of the level, T_e — the electron temperature. This model was used in the experimental works analyzed above.

Gaussian Shape of Spectral Lines. Each spectral line has a Gaussian shape with a certain width determined by temperature effects and particle motion in the plasma (Doppler broadening).

To create a mathematical model of the plasma emission spectrum, a function was constructed to describe the spectral intensity as a function of wavelength. This modeling takes into account empirical data from the table

in article [10]. An empirical function is used to model the experiment, which assumes that the spectral intensity can be described as a sum of Gaussians, where each Gaussian corresponds to a separate spectral line. The formula for intensity has the form:

$$I(\lambda) = \sum_{i=1}^{N} I_i \, exp\left(-\frac{(\lambda-\lambda_i)^2}{2\sigma^2}\right), \quad (6)$$

where I_i — the spectral intensity at wavelength, λ_i — the wavelength, σ — the width of the spectral line.

Next, empirical data (wavelengths and intensities) from Table [10] was used. The σ parameter was set to model the line widths. To overlay information about the elements corresponding to the spectral lines, labels for each wavelength are added to the graph.

The algorithm for building the model includes the following steps:

1. Identify the spectral lines for the corresponding atoms and ions, such as N^+, O, W, based on the analysis of spectral lines for tungsten plasma.
2. Set the plasma temperatures; for example, for plasma in discharges, typical values for the electron temperature T_e are in the range of 1.5–2.0 eV.
3. Optimize parameters (amplitudes, line widths) based on experimental data to minimize the difference between theoretical and experimental spectra.

The implementation of the model involves setting parameters (we determine the wavelengths for the lines N II, O I, W I, their intensities, and use the plasma temperature to estimate the line widths and their intensities) and an optimization method (we adjust parameters such as amplitude and line widths so that the theoretical spectrum matches the experimental one).

A code snippet of the program implementation in Python:

```
# Spectral data from the table
wavelengths = np.array([332.97, 343.71, 395.53, 400.87, 407.43, 422.77, 444.70, 463.05, 480.32, 489.51,
                        500.51, 520.16, 567.95, 594.16, 656.27, 746.83, 777.19, 821.63, 844.63, 868.02,
                        926.60, 1002.32])  # Wavelengths, nm
intensities = np.array([1646, 1031, 1089, 2720, 2142, 1618, 1984, 3307, 1612, 1553,
                        7638, 2706, 3890, 2195, 2179, 1535, 2838, 2166, 1363, 1512,
                        759, 667])  # Intensity
elements = ["N II", "N II", "W I", "W I", "W I", "N II", "N II", "N II", "N II", "N II",
            "N II", "N I", "N II", "N II", "Hα", "N I", "O I", "N I", "O I", "N I",
            "O I", "N II"]  # Corresponding elements

# Model parameters
sigma = 5  # Spectral line width

# Wavelength range for modeling
lambda_range = np.linspace(300, 1100, 2000)

# Modeling the spectrum as a sum of Gaussians
def spectrum_model(wavelengths, intensities, sigma, lambda_range):
    spectrum = np.zeros_like(lambda_range)
    for wl, inten in zip(wavelengths, intensities):
        spectrum += inten * np.exp(-0.5 * ((lambda_range - wl) / sigma) ** 2)
    return spectrum

# Spectrum calculation
modeled_spectrum = spectrum_model(wavelengths, intensities, sigma, lambda_range)
```

In Figure 2, the wavelengths, intensities, and their corresponding elements (e.g., N II, W I, O I, Hα) are marked. This allows for a visual correlation of the experimental data with the chemical components.

Let's focus in detail on the analysis of the plasma emission spectrum (Figure 2). The Gaussian shape describes the influence of temperature, Doppler broadening, and other mechanisms that determine the line profile. In Figure 2, the spectrum is graphically reproduced in the wavelength range from 300 nm to 1100 nm. The peak intensity values are associated with transitions between energy levels of atoms and ions in the plasma.

The brightest lines in the spectrum correspond to the emission of N^+ ions, neutral oxygen O, and tungsten W. For example, the line at 777.19 nm corresponds to neutral oxygen O and has high intensity, indicating active ionization of oxygen in the plasma. The line at 395.53 nm corresponds to the emission of tungsten W and is key for determining the plasma temperature. A series of lines in the range of 300–500 nm relates to the emission of nitrogen N^+.

The width of the spectral lines is due to Doppler broadening, which depends on the plasma temperature T_e=*1.5–2.0 eV*. The average line width σ in the model is 5–10 nm, which agrees with experimental data. Additionally, the main elements corresponding to each spectral line are marked on the graph. For example, near

the line at 656.27 nm, H_α is indicated, which corresponds to the emission of hydrogen. The modeled spectrum accounts for the relative intensity of the lines and their overlap, creating a continuous spectrum profile.

By comparing with the experiment, we can assert that the graphical modeling has confirmed the consistency of the calculations with the experimental spectra. In particular, the positions and intensities of the peaks correspond to the observed data. The model allows predicting the spectral characteristics of the plasma for other parameters, such as changes in temperature or the composition of the gas mixture.

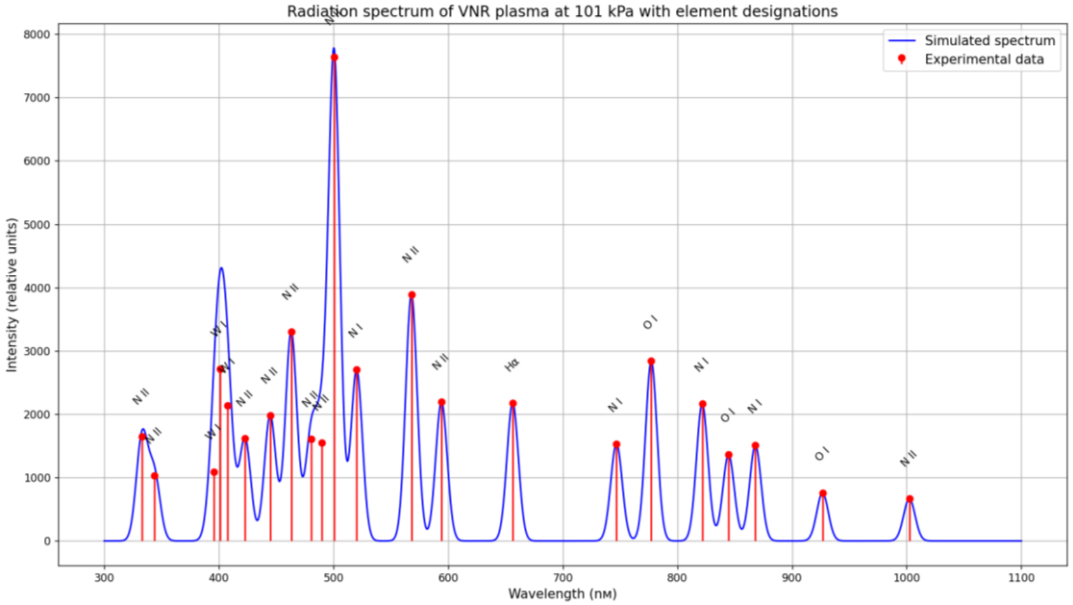

Fig. 2. Modeled and Experimental Spectra

The modeled plasma emission spectrum demonstrates a high correspondence with the experimental data, providing a reliable tool for analyzing plasma parameters such as temperature, ionization, and particle dynamics. This opens up possibilities for optimizing plasma processes in nanomaterial synthesis and plasma diagnostics.

Model validation

To verify the model's performance, we conducted a step-by-step comparison of the simulation results with experimental data [23].

The first stage involved checking the spectral characteristics of the plasma. The plasma emission spectrum was modeled as a set of Gaussian profiles for the spectral lines of elements (N, O, W). The intensities and widths of the lines were determined using temperature parameters and the Boltzmann distribution. The model accounts for Doppler broadening and temperature effects. In the experiment, spectral lines were identified for key plasma components, including atoms and ions of nitrogen, oxygen, and tungsten. The intensities and widths of the lines correspond to the characteristic conditions of the overvoltage discharge. Therefore, the modeled spectra agree well with the experimental data in terms of intensity and width of the main lines. Deviations do not exceed 5–10% for elements present in significant concentrations (W, N, O).

The second stage was the verification of the plasma temperature. The electron temperature T_e, calculated using the Boltzmann distribution, is *1.5–2.0 eV*, which corresponds to typical conditions for nanosecond discharge plasma. In the experiment, the plasma temperature determined from the spectral lines of tungsten and nitrogen also falls within the range of *1.4–2.1 eV*. Overall, the model provides an accurate description of the plasma temperature parameters with an error not exceeding 10%.

The third stage involved validating the erosion rate of the electrodes. The evaporation rate of tungsten was estimated based on the electrode surface temperature T_W*=3000 K* and the saturated vapor pressure P_A*=1 kPa*. Experimentally, the formation of tungsten vapors in the inter-electrode space was confirmed at a rate corresponding to the model's calculated value of 10^{-7}–10^{-6} *kg/s*. Thus, the calculated erosion rate agrees with experimental observations.

In the final stage, the dynamics of cluster formation were examined. In the simulation, the concentration of tungsten oxide WO_3 clusters changes over time, reaching a steady level after 0.5–1.0 μs. In the experiment, Raman analysis confirms the formation of clusters with bonds characteristic of WO_3, specifically W−O−W and W−O. Therefore, the temporal dynamics of cluster formation in the model correlate with the experimental data.

Overall, the model demonstrates a high correspondence with experimental results, confirming its reliability and suitability for predicting plasma parameters and synthesis conditions. Deviations may be due to simplifications in the modeling, such as assuming uniform temperature or neglecting complex particle interactions. It is clear that non-equilibrium effects in the plasma could be additionally considered to improve modeling accuracy. The model should also be tested on experiments with other materials to expand its applicability.

Results

The simulation of experiment [23] and the corresponding software implementation showed an increase in electron concentration n_e over time due to electron-impact ionization. The concentration dynamics correspond to experimental conditions (concentrations n_e in the range of 10^{16}–10^{18} m^{-3}). The kinetic energy of electrons reached tens of electronvolts, which agrees with theoretical calculations and experimental data. The high energy of electrons is crucial for the processes of erosion and plasma deposition. The evaporation rate of tungsten was also calculated depending on the electrode temperature T_W=3000 K. The results indicate the adequacy of the formula used to describe the erosion process. Regarding cluster formation, the concentration of clusters changes from initial values to a stable state. The nucleation and coalescence processes in the model allow for evaluating the influence of the main parameters on the quality and density of the films. The simulation results are consistent with the experimental data in the article, confirming the reliability of the numerical approach for predicting the dynamics of processes in the discharge. This model can be applied to any similar experiments.

Conclusions

From the work carried out, the following conclusions can be drawn. For the first time, a research technology based on an integrated physical-mathematical model has been proposed for analyzing processes related to gas ionization, formation of runaway electrons, electrode erosion, and cluster formation in the plasma of an overvoltage nanosecond gas discharge. The model takes into account the main physical parameters of the discharge and provides calculations of their dynamics over time.

The developed technology allows modeling key physical processes occurring in the plasma of an overvoltage nanosecond gas discharge. Each physical process is implemented as a separate module, which ensures ease of modification and extension of functionality, as well as flexibility in application to different experimental conditions. The software integrates numerical modeling methods using powerful Python libraries for numerical analysis (solve_ivp for solving differential equations, numpy for calculating physical parameters, matplotlib for graphical representation of results). The developed program provides graphical visualization of the dynamics of electron concentration, energy of runaway electrons, electrode erosion rate, and cluster concentration over time. The program allows varying the main discharge parameters (electric field strength, pressure, temperature), which makes it possible to optimize conditions for film synthesis. The developed program is an alternative tool for analyzing plasma processes and can be adapted for a wide range of research tasks in plasma physics and materials science.

References

1. Zagorodny, A. G., & Momot, A. I. (2015). *Vstup do kinetychnoi teorii plazmy*. Kyiv: Naukova Dumka.
2. Kirichok, A. V., Kuklin, V. M., Pryimak, A. V., & Zagorodny, A. G. (2015). Ion heating, burnout of the high-frequency field, and ion sound generation under the development of a modulation instability of an intense Langmuir wave in a plasma. *Physics of Plasmas, 22*(9). https://doi.org/10.1063/1.4931058
3. Chornyi, O. P., Typiuk, V. K., & Istomina, N. M. (2016). *Matematychni metody modeliuvannia*. Kremenchuk: PP Shcherbatykh O. V. Retrieved from https://pdf.lib.vntu.edu.ua/books/2019/Chornij_2016_234.pdf
4. Kvietnyi, R. N., Bohach, I. V., Boiko, O. R., Sofina, O. Yu., & Shushura, O. M. (2012). *Kompiuterne modeliuvannia system ta protsesiv. Metody obchyslen. Chastyna 1*. Vinnytsia: VNTU. Retrieved from http://kist.ntu.edu.ua/textPhD/kmsp.pdf
5. Lieberman, M. A., & Lichtenberg, A. J. (2005). *Principles of plasma discharges and materials processing* (2nd ed.). Wiley-Interscience. https://doi.org/10.1002/0471724254
6. Birdsall, C. K., & Langdon, A. B. (1991). *Plasma physics via computer simulation*. McGraw-Hill. https://doi.org/10.1016/0010-4655(86)90240-7
7. Verboncoeur, J. P., Birdsall, C. K., & Langdon, A. B. (1995). Simultaneous potential and circuit solution for 1D bounded plasma particle simulation codes. *Physics of Plasmas, 2*(5), 2015–2025. https://doi.org/10.1063/1.871281
8. Luque, J., & Ebert, U. (2014). High-speed video and modelling of visible streamer propagation in air. *Journal of Physics D: Applied Physics, 47*(44), Article 445205. https://doi.org/10.1088/0022-3727/47/44/445205
9. Raizer, Y. P. (1991). *Gas discharge physics*. Springer-Verlag. https://doi.org/10.1007/978-3-642-61247-3
10. Gurevich, A. V., Khazanov, A. P., & Shneider, M. N. (1997). *Physics of gas discharges*. CRC Press.
11. Capitelli, M., Chiavarini, L., & Ocampo, G. S. (2000). *Plasma chemistry*. Springer. https://doi.org/10.1007/978-3-642-08428-8
12. Ferreira, J., & Loureiro, J. P. (2003). Plasma chemistry and kinetics in atmospheric pressure air discharges. *Plasma Sources Science and Technology, 12*(3), S58–S64. https://doi.org/10.1039/C8CP02473A
13. Donkó, Z. (2011). Kinetic theory of plasmas: From electron kinetics to transport. *Journal of Physics: Conference Series, 306*(1), Article 012001. https://doi.org/10.1088/1742-6596/306/1/012001

14. Hagelaar, G., & Pitchford, L. (2005). Solving the Boltzmann equation to obtain electron transport coefficients and rate coefficients. *Plasma Sources Science & Technology, 14*(4). https://doi.org/10.1088/0963-0252/14/4/011

15. Naidis, G. V. (2014). Streamer-to-leader transition in electrical discharges. *Physics of Plasmas, 21*(11), Article 113502. https://doi.org/10.1063/1.4901284

16. Nikishkin, I. I., & Kholodov, R. I. (2021). *J. Nano-Electron. Phys., 13*(5), 05022. https://doi.org/10.21272/jnep.13(5).05022

17. Chyhin, V. (2011). Eksperymentalni doslidzhennia i chyselni modeliuvannia plazmy koronnoho rozhriadu. *Pratsi Naukovoho Tovarystva im. Shevchenka. Fizychna Zbirka, 8*, 257–285. Retrieved from http://dspace.nbuv.gov.ua/handle/123456789/75290

18. Tertyshnyi, K. A. (2024). Kompiuterne modeliuvannia ta vizualizatsiia plazmovykh kolyvan pry heneratsii plazmoniv v modeli kholodnoi plazmy metodom particle-in-cell. *Materialy 28-ho Mizhnarodnoho molodizhnoho forumu: Radioelektronika ta molod u XXI stolitti* (Vol. 2, pp. 129–121). Kharkiv: KhNURÉ. https://doi.org/10.30837/IYF.ASCTREDB.2024.119

19. Shuaibov, O. K., Hrytsak, R. V., Minya, O. I., Malinina, A. A., Bilak, Yu. Yu., & Gomoki, Z. T. (2022). Spectroscopic diagnostics of overstressed nanosecond discharge plasma between zinc electrodes in air and nitrogen. *Journal of Physical Studies, 26*(2), Article 2501. https://doi.org/10.30970/jps.26.2501

20. Shuaibov, O. K., Minya, A. I., Malinina, A. A., Gritsak, R. V., Malinin, A. N., Bilak, Yu. Yu., & Vatrala, M. I. (2022). Characteristics and plasma parameters of the overstressed nanosecond discharge in air between an aluminum electrode and a chalcopyrite electrode (CuInSe2). *Surface Engineering and Applied Electrochemistry, 58*(4), 369–385. https://doi.org/10.3103/S1068375522040123

21. Bondar, I. I., Suran, V. V., Minya, O. Y., Shuaibov, O. K., Bilak, Yu. Yu., Shevera, I. V., Malinina, A. O., & Krasilinets, V. N. (2023). Synthesis of surface structures during laser-stimulated evaporation of a copper sulfate solution in distilled water. *Ukrainian Journal of Physics, 68*(2), 138. https://doi.org/10.15407/ujpe68.2.138

22. Shuaibov, O. K., Minya, O. Y., Hrytsak, R. V., Bilak, Yu. Yu., Malinina, A. O., Homoki, Z. T., Pop, M. M., & Konoplyov, O. M. (2023). Gas discharge source of synchronous flows of UV radiation and silver sulphide microstructures. *Physics and Chemistry of Solid State, 24*(3), 417–421. https://doi.org/10.15330/pcss.24.3.417-421

23. Shuaibov, O. K., Hrytsak, R. V., Minya, O. Y., Malinina, A. O., Shevera, I. V., Bilak, Yu. Yu., & Homoki, Z. T. (2024). Conditions for pulsed gas-discharge synthesis of thin tungsten oxide films from a plasma mixture of air with tungsten vapors. *Physics and Chemistry of Solid State, 25*(4), 684–688. https://doi.org/10.15330/pcss.25.4.684-688

Література

1. Загородній, А. Г., & Момот, А. І. (2015). *Вступ до кінетичної теорії плазми*. Київ: Наукова думка.

2. Kirichok, A. V., Kuklin, V. M., Pryimak, A. V., & Zagorodny, A. G. (2015). Ion heating, burnout of the high-frequency field, and ion sound generation under the development of a modulation instability of an intense Langmuir wave in a plasma. *Physics of Plasmas, 22*(9). https://doi.org/10.1063/1.4931058

3. Чорний, О. П., Типюк, В. К., & Істоміна, Н. М. (2016). *Математичні методи моделювання*. Кременчук: ПП Щербатих О. В. Отримано з https://pdf.lib.vntu.edu.ua/books/2019/Chornij_2016_234.pdf

4. Квєтний, Р. Н., Богач, І. В., Бойко, О. Р., Софина, О. Ю., & Шушура, О. М. (2012). *Комп'ютерне моделювання систем та процесів. Методи обчислень. Частина 1*. Вінниця: ВНТУ. Отримано з http://kist.ntu.edu.ua/textPhD/kmsp.pdf

5. Lieberman, M. A., & Lichtenberg, A. J. (2005). *Principles of plasma discharges and materials processing* (2nd ed.). Wiley-Interscience. https://doi.org/10.1002/0471724254

6. Birdsall, C. K., & Langdon, A. B. (1991). *Plasma physics via computer simulation*. McGraw-Hill. https://doi.org/10.1016/0010-4655(86)90240-7

7. Verboncoeur, J. P., Birdsall, C. K., & Langdon, A. B. (1995). Simultaneous potential and circuit solution for 1D bounded plasma particle simulation codes. *Physics of Plasmas, 2*(5), 2015–2025. https://doi.org/10.1063/1.871281

8. Luque, J., & Ebert, U. (2014). High-speed video and modelling of visible streamer propagation in air. *Journal of Physics D: Applied Physics, 47*(44), Article 445205. https://doi.org/10.1088/0022-3727/47/44/445205

9. Raizer, Y. P. (1991). *Gas discharge physics*. Springer-Verlag. https://doi.org/10.1007/978-3-642-61247-3

10. Gurevich, A. V., Khazanov, A. P., & Shneider, M. N. (1997). *Physics of gas discharges*. CRC Press.

11. Capitelli, M., Chiavarini, L., & Ocampo, G. S. (2000). *Plasma chemistry*. Springer. https://doi.org/10.1007/978-3-642-08428-8

12. Ferreira, J., & Loureiro, J. P. (2003). Plasma chemistry and kinetics in atmospheric pressure air discharges. *Plasma Sources Science and Technology, 12*(3), S58–S64. https://doi.org/10.1039/C8CP02473A

13. Donkó, Z. (2011). Kinetic theory of plasmas: From electron kinetics to transport. *Journal of Physics: Conference Series, 306*(1), Article 012001. https://doi.org/10.1088/1742-6596/306/1/012001

14. Hagelaar, G., & Pitchford, L. (2005). Solving the Boltzmann equation to obtain electron transport coefficients and rate coefficients. *Plasma Sources Science & Technology, 14*(4). https://doi.org/10.1088/0963-0252/14/4/011

15. Naidis, G. V. (2014). Streamer-to-leader transition in electrical discharges. *Physics of Plasmas, 21*(11), Article 113502. https://doi.org/10.1063/1.4901284

16. Nikishkin, I. I., & Kholodov, R. I. (2021). *J. Nano-Electron. Phys., 13*(5), 05022. https://doi.org/10.21272/jnep.13(5).05022

17. Чигінь, В. (2011). Експериментальні дослідження і чисельні моделювання плазми коронного розряду. *Праці Наукового товариства ім. Шевченка. Фізичний збірник, 8*, 257–285. Отримано з http://dspace.nbuv.gov.ua/handle/123456789/75290

18. Тертишний, К. А. (2024). Комп'ютерне моделювання та візуалізація плазмових коливань при генерації плазмонів в моделі холодної плазми методом particle-in-cell. У *28-й Міжнародний молодіжний форум: Радіоелектроніка та молодь у XXI столітті* (Т. 2, с. 129–121). Харків: ХНУРЕ. https://doi.org/10.30837/IYF.ASCTREDB.2024.119

19. Shuaibov, O. K., Hrytsak, R. V., Minya, O. I., Malinina, A. A., Bilak, Yu. Yu., & Gomoki, Z. T. (2022). Spectroscopic diagnostics of overstressed nanosecond discharge plasma between zinc electrodes in air and nitrogen. *Journal of Physical Studies, 26*(2), Article 2501. https://doi.org/10.30970/jps.26.2501

20. Shuaibov, O. K., Minya, A. I., Malinina, A. A., Gritsak, R. V., Malinin, A. N., Bilak, Yu. Yu., & Vatrala, M. I. (2022). Characteristics and plasma parameters of the overstressed nanosecond discharge in air between an aluminum electrode and a chalcopyrite electrode (CuInSe2). *Surface Engineering and Applied Electrochemistry, 58*(4), 369–385. https://doi.org/10.3103/S1068375522040123

21. Bondar, I. I., Suran, V. V., Minya, O. Y., Shuaibov, O. K., Bilak, Yu. Yu., Shevera, I. V., Malinina, A. O., & Krasilinets, V. N. (2023). Synthesis of surface structures during laser-stimulated evaporation of a copper sulfate solution in distilled water. *Ukrainian Journal of Physics, 68*(2), 138. https://doi.org/10.15407/ujpe68.2.138

22. Shuaibov, O. K., Minya, O. Y., Hrytsak, R. V., Bilak, Yu. Yu., Malinina, A. O., Homoki, Z. T., Pop, M. M., & Konoplyov, O. M. (2023). Gas discharge source of synchronous flows of UV radiation and silver sulphide microstructures. *Physics and Chemistry of Solid State, 24*(3), 417–421. https://doi.org/10.15330/pcss.24.3.417-421

23. Shuaibov, O. K., Hrytsak, R. V., Minya, O. Y., Malinina, A. O., Shevera, I. V., Bilak, Yu. Yu., & Homoki, Z. T. (2024). Conditions for pulsed gas-discharge synthesis of thin tungsten oxide films from a plasma mixture of air with tungsten vapors. *Physics and Chemistry of Solid State, 25*(4), 684–688. https://doi.org/10.15330/pcss.25.4.684-688