МАТЕМАТИЧНЕ МОДЕЛЮВАННЯ В ПРИРОДНИЧИХ НАУКАХ ТА ІНФОРМАЦІЙНІ ТЕХНОЛОГІЇ

MATHEMATICAL MODELING IN NATURAL SCIENCES AND INFORMATION TECHNOLOGIES

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PLASMA PROCESSES IN OVERVOLTAGE NANOSECOND DISCHARGE: NUMERICAL MODELING BY MONTE CARLO METHOD AND SOFTWARE IMPLEMENTATION IN PYTHON

ПЛАЗМОВІ ПРОЦЕСИ У ПЕРЕНАПРУЖЕНИХ НАНОСЕКУНДНИХ РОЗРЯДАХ: ЧИСЕЛЬНЕ МОДЕЛЮВАННЯ МЕТОДОМ МОНТЕ-КАРЛО ТА ПРОГРАМНА РЕАЛІЗАЦІЯ НА PYTHON

The article discusses the use of the Monte Carlo method for numerical modeling of plasma processes in overvoltage nanosecond discharges. The principle of the method, its algorithm, and key aspects of the software implementation are described in detail, in particular, the use of Python using the NumPy and SciPy libraries to model particle trajectories, collision probabilities, and energy distributions. The main goal of the work was to study plasma parameters, such as the electron energy distribution function (EEDF), electron temperature, plasma density, and optical characteristics, including spectral dependences of radiation. The work analyzed the behavior of electrons in gas mixtures under various conditions, including changes in the electric field E/N and pressure. The simulation results showed a high correlation with experimental data, confirming the effectiveness of the Monte Carlo method for analyzing microscopic processes in plasma. The study includes an analysis of alternative plasma modeling methods, such as magnetohydrodynamic models, models based on the Boltzmann equation (BOLSIG+), and hybrid approaches. The development of a numerical model of plasma processes is important in the context of the rapid development of computing technology, which allows performing complex calculations with high accuracy. This opens up new opportunities for the application of plasma technologies in industry, including the development of energy-efficient devices and innovative materials. Thus, the work has both fundamental and applied significance, contributing to the solution of urgent problems of modern science and technology.

The practical significance of the work lies in the application of the results to create thin films, in particular chalcopyrites, in photovoltaic devices. Plasma modeling in overvoltage discharges shows significant potential for optimizing the synthesis conditions of nanomaterials with controlled properties. In the future, the proposed model can be adapted for additional tasks, including the influence of a magnetic field and the analysis of spectral characteristics. The results of the work confirm the importance of numerical modeling for the study of plasma processes and their further use in high-tech applications, in particular for the development of plasma methods for the synthesis of nanomaterials.

***Keywords**: Monte Carlo, modeling, spectrum, nanomaterials, python.*

У статті розглянуто використання методу Монте-Карло для чисельного моделювання плазмових процесів у перенапружених наносекундних розрядах. Детально описано принцип роботи методу, його алгоритм та ключові аспекти програмної реалізації, зокрема застосування Python із використанням бібліотек NumPy та SciPy для моделювання траєкторій частинок, ймовірностей зіткнень та енергетичних розподілів.

Основною метою роботи було дослідження параметрів плазми, таких як функція розподілу енергії електронів (EEDF), температура електронів, щільність плазми, а також оптичні характеристики, включаючи спектральні залежності випромінювання. У роботі проаналізовано поведінку електронів у газових сумішах за різних умов, включаючи зміни електричного поля E/N та тиску. Результати моделювання показали високу кореляцію з експериментальними даними, підтверджуючи ефективність методу Монте-Карло для аналізу мікроскопічних процесів у плазмі.

Дослідження включає аналіз альтернативних методів моделювання плазми, таких як магнітогідродинамічні моделі, моделі на основі рівняння Больцмана (BOLSIG+), а також гібридні підходи. Розробка чисельної моделі плазмових процесів є важливою у контексті швидкого розвитку обчислювальної техніки, що дає змогу виконувати складні розрахунки з високою точністю. Це відкриває нові можливості для застосування плазмових технологій у промисловості, включаючи розробку енергоефективних пристроїв та інноваційних матеріалів. Таким чином,

робота має як фундаментальне, так і прикладне значення, сприяючи вирішенню актуальних завдань сучасної науки та техніки.

Практичне значення роботи полягає у застосуванні результатів для створення тонких плівок, зокрема халькопіритів, у фотоелектричних пристроях. Моделювання плазми у перенапружених розрядах показує значний потенціал для оптимізації умов синтезу наноматеріалів із контрольованими властивостями. У майбутньому, запропонована модель може бути адаптована для додаткових задач, включаючи вплив магнітного поля та аналіз спектральних характеристик. Результати роботи підтверджують важливість чисельного моделювання для вивчення плазмових процесів та подальшого використання у високотехнологічних застосуваннях, зокрема для розвитку плазмових методів синтезу наноматеріалів.

***Ключові слова**: Монте-Карло, моделювання, спектр, наноматеріали, python.*

Problem's Formulation

The study of plasma processes in overdriven nanosecond discharges is a complex task that requires an understanding of the interactions between electrons, ions, and neutral particles in gaseous environments. These processes are non-equilibrium in nature and are accompanied by intricate microscopic phenomena, such as collisions, ionization, excitation, and particle recombination.

Modern experimental methods allow for the acquisition of extensive information about plasma; however, their capabilities are limited by the complexity of discharge conditions, the high speed of processes, and significant computational costs associated with data analysis. Traditional analytical and hydrodynamic models do not provide sufficient accuracy for describing non-equilibrium processes.

The need to develop numerical approaches that can provide a detailed description of plasma processes is particularly important for nanomaterial synthesis technologies, such as thin films based on chalcopierites, which are used in photovoltaic devices. One of the most effective approaches for modeling such processes is the Monte Carlo method, which allows for the consideration of the probabilistic nature of particle interactions, as well as their trajectories and energy characteristics. However, the application of the Monte Carlo method requires the development of specialized algorithms and software tailored to plasma physics problems. Additionally, there is a need for the validation of numerical results through comparison with experimental data, which is complicated by the large number of plasma parameters that must be taken into account.

Thus, the problem arises of creating an effective plasma model for overdriven nanosecond discharges that would allow for a detailed study of energetic processes, optimization of discharge parameters and nanomaterial synthesis, as well as ensuring high accuracy and computational efficiency.

Analysis of recent research and publications

Modeling plasma processes occupies a central role in understanding plasma behavior. In particular, the Monte Carlo method (MCS) deserves special attention as a powerful tool for numerically simulating various plasma processes, including those in overdriven nanosecond discharges, as demonstrated by numerous studies. For instance, the book [1] highlights the importance of MCS for modeling thermodynamic properties and particle interactions in the presence of local or external fields, such as in thin-film deposition processes via Plasma-Enhanced Chemical Vapor Deposition (PECVD). This approach enables detailed examination of interactions in gas phases; however, as noted, realistic modeling of complex plasma processes requires improvements in algorithms and computational efficiency. Similarly, the study [2] explored Monte Carlo methods for modeling electron-liquid interactions, which is important for understanding processes like hydrated electron and radical formation in plasma discharges. While the results are promising, questions remain regarding the accuracy of modeling such processes under different energy regimes, particularly in low-energy electron collisions, which are crucial for overdriven discharge characteristics. The application of Monte Carlo methods to plasma modeling in Electron Cyclotron Resonance Ion Sources (ECRIS) in [3] shows how these methods can be used to describe spatial and energy distributions of particles. However, while this approach is fast and efficient for specific conditions, it also highlights the need for new methods for more accurate plasma environment descriptions in complex discharges with strong electric and magnetic fields. Other research, such as the review in [4], illustrates the potential of using MCS for modeling conducting polymer composites, yet these methods are limited when it comes to complex plasma systems where particle-material

interactions require more specialized approaches. This emphasizes the importance of enhancing numerical methods for simulating such multiphase systems, particularly under high energy conditions. The study of plasma microphysics, as shown in [5], using MCS for generating relativistic electron-positron beams in accelerators, offers insights into possible advancements in modeling high-density plasmas. However, significant issues remain regarding the accuracy of these models under specific conditions, such as extreme astrophysical environments or intense overdriven discharges in laboratory settings. Finally, research [6] on molecular-kinetic simulations of fermionic path integrals confirms the need for a deeper understanding of momentum distribution in non-ideal electron gases, which is also highly relevant for modeling plasma processes in overdriven discharges. Nonetheless, there remains the question of improving these models to account for short-lived and high-frequency plasma oscillations. Thus, despite the successful application of the Monte Carlo method in numerical modeling of various plasma processes, including overdriven nanosecond discharges, significant unresolved issues remain related to computational efficiency, accuracy, and scalability of models. This underscores the relevance of developing new algorithms and software implementations capable of accounting for the complex physical conditions present in such processes.

Numerical simulation of plasma processes is a crucial tool for studying complex physical phenomena, especially in overdriven nanosecond discharges, which require improvements in existing methods and models to achieve more accurate results. In article [7], two key aspects of plasma process numerical modeling are discussed. The first aspect pertains to modeling physical processes prior to simulation, where magnetohydrodynamic (MHD) models are used, taking into account nonequilibrium processes (TNE), including entropy generation rates. This approach allows for the physical correctness of the model to be assessed through test problems, such as the Orszag-Tang vortex. The second aspect concerns the analysis of nonequilibrium states after simulation, particularly using non-conservative kinetic moments to describe instabilities such as Richtmyer-Meshkov (RMI), demonstrating the influence of the magnetic field on TNE effects. The identified dependencies point to the need for further research to optimize models describing complex plasma phenomena under such conditions. In work [8], molecular dynamics modeling of hydrogen plasma is considered, focusing on the relaxation process toward equilibrium. Since precise experimental data is lacking, such simulations serve as "idealized computational experiments." The approaches described in this paper allow for the correctness of numerical simulations to be assessed through the developed analytical equilibrium model, confirming the importance of integrating molecular dynamics and analytical methods for accurate results. Article [9] proposes a new physically grounded computational model, DEIVI, which predicts material ablation under nanosecond laser radiation. This approach integrates various physical processes, including laser absorption, heat exchange, and evaporation, using models to describe the dynamics of melting, vapor, and gas. Despite a high level of verification, this approach underscores the need for further refinement of models for more accurate ablation predictions in real experimental setups. Work [10] discusses numerical modeling of low-temperature nonequilibrium plasma in dielectric barrier discharge in air. The developed model describes the spatiotemporal structure of plasma, taking into account numerous kinetic phenomena and plasma-chemical reactions. It allows for the investigation of plasma ignition and development stages, but an important task remains the refinement of parameters such as streamer formation rate and particle density distribution dynamics. Article [11] analyzes methods for determining the minimum reflection characteristic during surface plasmon resonance. The proposed new average line method significantly reduces errors compared to traditional polynomial methods and holds considerable potential for improving accuracy in signal processing during surface plasmon resonance analysis. However, for widespread application of this method, additional factors that may influence the accuracy of results in real conditions need to be considered. In article [12], elementary processes of charged particle interactions in an electron beam are studied using a one-dimensional particle-in-cell code. This study allows for the analysis of electron-positron and electron-proton gas oscillations, revealing relaxation times and spectral oscillation distributions that match theoretical estimates. However, for further model development, it is necessary to account for more complex physical interactions that may occur across a broader range of parameters.

In general, numerical modeling of plasma processes, particularly in overdriven nanosecond discharges, remains a relevant challenge due to the need for integrating cutting-edge physical models and

enhancing existing methods. Identifying optimal numerical approaches that can effectively solve these complex problems is a crucial step towards achieving accurate results in plasma process research.

Experimental studies have also been conducted in a number of scientific works that require further modeling and processing of the obtained data. In works [13–18], various aspects of overdriven nanosecond discharges and their application for the synthesis of thin films and nanostructures are analyzed. In [13], spectral characteristics of the plasma between zinc electrodes and the synthesis of nanostructured films made of zinc, zinc oxide, and zinc nitride are studied. In [14], plasma between aluminum and chalcopyrite electrodes is examined for the synthesis of CuAlInSe2 films and the determination of key plasma parameters. In [15], the influence of laser radiation on the formation of structured films from an aqueous copper sulfate solution is analyzed. In [16], the discharge features in nitrogen between electrodes made of silver sulfide (Ag2S) are described, enabling the generation of UV radiation and microstructured films. In [17], a method for the synthesis of WO3 films in a gas-phase mixture of "Air-W" without the use of vacuum technology is proposed. The article [18] investigates the electrophysical properties of thin films based on the superionic conductor Ag_2S, synthesized by a gas discharge deposition method in an air atmosphere. The authors describe the film creation process, analyze their electrical conductivity and structure, and consider the potential use of these materials in modern electronic devices such as sensors and batteries. Numerical modeling of processes is essential for all these works due to the complexity and high computational demands of the experiments.

Formulation of the study purpose

The aim of this research is to develop a numerical model of plasma processes in overcharged nanosecond discharges using the Monte Carlo method. Specifically, the objectives of the work are:

- To develop a simulation algorithm that describes the dynamics of particles in the plasma, specifically electrons and ions, taking into account processes such as collisions, ionization, excitation, and recombination.
- Development of software based on Python for performing numerical calculations, including the computation of electron energy distribution, temperature, plasma density, and other parameters that describe the plasma state.
- Validation of the model by comparing the obtained results with experimental data regarding the parameters of nanosecond discharges in gas mixtures.
- Optimization of plasma process parameters for the synthesis of thin films, particularly chalcopyrites, for use in photovoltaic devices.
- Determination of the prospects and limitations of the Monte Carlo method for modeling plasma processes, and evaluation of the potential application of the developed model in other areas of plasma physics and materials technology.

The main result of the work is the improvement of numerical modeling for precise analysis of plasma processes in high-precision and complex discharge conditions.

Presenting main material

Analysis of methods and models. Processes in plasma, similar to those described in [14], can be modeled using several approaches, depending on the objectives and available resources. The main alternative modeling methods include Monte Carlo simulations, magnetohydrodynamic (MHD) approaches, kinetic equation-based modeling, density functional theory (DFT) methods, hybrid models, and the use of commercial or open-source software.

Monte Carlo numerical modeling allows for the simulation of particle behavior in plasma, taking into account the probabilistic nature of their interactions. Among the advantages of the method, it is worth noting the ability to detail microprocesses such as collisions, ionization, and recombination. Additionally, it is well-suited for small plasma volumes and rarefied collisions. However, this method has high computational complexity for large systems. Currently, it is used for precise analysis of electron and ion collisions, including microerosion of electrodes.

MHD models [19] describe plasma as a continuous medium, taking into account electromagnetic and hydrodynamic effects. These models are well-suited for large-scale systems, where the movement of plasma in the discharge gap needs to be considered, and they also account for the influence of magnetic fields. However, it should be noted that they are less accurate for simulating microscopic

processes, such as those at the electron level. They are primarily used for the analysis of large discharge volumes or fast gasdynamic processes.

Kinetic equation-based modeling [20] relies on solving conservation equations (mass, energy, momentum) and kinetic equations. This approach allows the description of dynamic changes in the concentration of ions, electrons, and neutral particles, taking into account the influence of chemical reactions, dissociation, and ionization. However, the method does not fully account for the details of energy distribution among particles, which is a limitation. It is primarily used for analyzing the chemical composition of plasma and changes in its properties over time.

Modeling particle interactions using quantum mechanical methods [21], such as first-principles calculations (or DFT), is one of the most accurate approaches for describing processes at the atomic and molecular levels. However, it has limitations for small volumes due to computational complexity. It is often used for analyzing microscopic processes at the energy level and transitions, especially in chalcopirites.

Hybrid models combine kinetic models (for fast particles, such as electrons) with MHD approaches (for ions and neutral particles) [22]. This aspect allows for the consideration of different time and spatial scales and helps determine the optimal balance between accuracy and computation speed. Regarding disadvantages, the complexity of setting up the models and integrating various approaches should be noted. Hybrid models are used for simulating plasma processes where both macroscopic and microscopic effects are important.

As for the use of commercial or open-source programs, some of them, like COMSOL Multiphysics, are better suited for MHD and kinetic modeling; for Particle-in-Cell (PIC) models, programs like XOOPIC or OpenFOAM are advantageous; for numerically solving the Boltzmann equation, BOLSIG+ from the Boltzmann Solver Packages is recommended.

Clearly, the choice of method depends on the required accuracy, plasma volume, time and spatial scales, and computational resources. If the goal is to study the energy distribution of electrons, the Boltzmann equation is the most suitable. For analyzing large, complex systems, it is advisable to use MHD modeling or hybrid approaches.

Below is a comparative table of the main methods for modeling plasma processes:

Table 1. Comparison of the main methods for modeling plasma processes

Method	**Key Characteristics**	**Advantages**	**Disadvantages**	**Typical Applications**
Monte Carlo Method	Probabilistic modeling of particle behavior	- Detailed collision modeling - Flexibility in calculations - Realistic process representation	- High computational costs - Difficult to scale for large systems	Study of microprocesses: ionization, collisions, erosion
MHD Models	Modeling plasma as a continuous medium with electromagnetic effects	- Large-scale description - Consideration of magnetic and hydrodynamic phenomena	- Low accuracy at the level of individual particles - Limited microprocess details	Analysis of gasdynamic phenomena in large discharge volumes
Kinetic Equations	Calculation of particle concentration and energy changes over time	- Suitable for chemical plasma analysis - Simple implementation for many tasks	- Ignores details of energy distribution - Less accuracy in fast particle dynamics	Plasma composition changes, chemical product synthesis

Continue of the table 1

Quantum Mechanics (DFT)	Detailed analysis of interactions at the atomic and molecular level	- Maximum accuracy - Ability to describe energy levels and transitions	- Low performance for large systems - Limited by molecular complexity	Energy levels, electronic transitions, microprocesses
Hybrid Models	Combination of kinetic and MHD methods for different plasma components	- Balance between detail and scale - Consideration of plasma's multilayer structure	-Complex implementation - High computational requirements	Large systems requiring detailed process modeling
Particle-in-Cell (PIC)	Simulation of particle motion in electromagnetic fields based on Maxwell's equations	- Effective for plasma flows - High accuracy in microanalysis	- Limited performance for high-density particle systems - Requires significant computational resources	Plasma flows, electron interactions
BOLSIG+ (Boltzmann Equation Solver)	Numerical solution of the Boltzmann equation for the electron energy distribution function	- Accurate modeling of electron energy characteristics - Suitable for collision and spectral analysis	- Applicable only to individual particles (electrons) -Ignores macroprocesses	Electron process analysis, excitation, ionization
COMSOL Multiphysics	Integration of various approaches in multiphysics systems (MHD, heat transfer, chemical reactions)	- Versatility - Intuitive interface - Multifunctionality	- Expensive license - High computational requirements	Various modeling aspects: plasma, heat transfer, chemical processes

After conducting a thorough analysis, the following conclusions were made as recommendations for usage. To model energy processes in plasma, it is convenient to use BOLSIG+ or the Monte Carlo method. For large-scale analysis, MHD models or COMSOL Multiphysics are suitable, while for high-precision calculations at the atomic level, quantum mechanical methods should be employed.

Modeling and Software Implementation. In this scientific work, the Monte Carlo method was chosen for the implementation of the task. The idea of the method lies in the statistical modeling of trajectories of a large number of particles (electrons, ions), considering their motion, collisions, and energy losses. Each particle is modeled separately, and average values are determined as statistics from all particles.

The algorithm of the method. The input data consists of plasma parameters (electron temperature T_e, electron density n_e, gas pressure P, and gas mixture composition (component concentrations)). The physical parameters selected include collision cross-sections σ(E) for various processes (elastic collisions, ionization, excitation, etc.), excitation potential E_{ex}, ionization potential E_{ion} for each component, and the electric field E. As for the modeling parameters, the number of particles $N_{particles}$, the maximum simulation time t_{max}, and the time step Δtwere chosen.

Steps of the simulation algorithm:

Step 1: Initialization

- Determine the initial positions and velocities of the particles.
- Assign each particle an initial energy corresponding to the Maxwell-Boltzmann distribution function.

Step 2: Process Selection

- Determine the collision probabilities for each type of process $P_i = n\sigma_i v\Box t$, where:
  - n — the concentration of target particles.
  - σ_i — the cross-section of process \(i\).
  - v — the particle velocity.
- Generate a random number$r \in [0,1]$ and compare it with the total collision probability $P = \sum P_i$, to determine the type of process:
  - If $r < P_{elastic}$, conduct an elastic collision.
  - If $P_{elastic} \le r < P_{elastic} + P_{ionization}$, conduct ionization..
  - And so on.

Step 3: Energy Update

- For each type of collision, adjust the particle's energy:
  - Elastic collision: the particle's energy changes slightly (due to energy transfer).
  - Ionization: energy decreases by Eion, and a new electron is added.
  - Excitation: energy decreases byE_{ex}.

Step 4: Update the trajectory.

- The motion of a particle in an electric field:

$$r(t+\Delta t) = r(t) + v(t)\Delta t; \tag{1}$$

$$v(t+\Delta t) = v(t) + \frac{qE}{m}\Delta t, \tag{2}$$

where q is the charge of the particle, and m is the mass of the particle.

Step 5: Repetition

- Repeat steps 2–4 for each particle until tmax is reached or particles are exhausted.

The obtained results should provide information about the energy distribution of electrons, i.e., determine the energy distribution function *f(E)* by counting the number of electrons in each energy interval. The plasma parameters should be determined, including the effective electron temperature

$$T_e = \frac{2}{3}\langle E \rangle$$

and the ionization level

$$\alpha = \frac{n_{ion}}{n_{total}}.$$

To provide the emission spectra, that is, the intensity of spectral lines associated with the excitation of atoms and molecules.

For the software implementation of the simulation process, Python (with the NumPy and SciPy libraries) [23] was chosen, which allowed obtaining the electron energy distribution, ionization coefficients, emission spectra, and other important parameters for plasma process analysis. A fragment of the developed program code is shown below:

```
# Function to generate initial electron velocities (Maxwell-Boltzmann distribution)
def initialize_velocities(T, N):
v_th = np.sqrt(2 * k_B * T / m)
vx = np.random.normal(0, v_th, N)
vy = np.random.normal(0, v_th, N)
vz = np.random.normal(0, v_th, N)
   return vx, vy, vz

# Function to calculate collision probabilities
def compute_collision_probabilities(v, sigma, n, dt):
   return n * sigma * v * dt

# Initialization of particles
```

```
vx, vy, vz = initialize_velocities(T_e, N_particles)
energies = 0.5 * m * (vx**2 + vy**2 + vz**2) / q  # Energy of electrons in eB
positions = np.zeros((N_particles, 3))  # Initial coordinates

# Saving the results
energy_history = []
time = 0
ionization_events = 0

# Main Monte Carlo loop
while time <t_max:
   time += dt
   # Electron velocity
v_magnitude = np.sqrt(vx**2 + vy**2 + vz**2)

   # Collision probabilities
P_el = compute_collision_probabilities(v_magnitude, sigma_el, n_gas, dt)
P_ex = compute_collision_probabilities(v_magnitude, sigma_ex, n_gas, dt)
P_ion = compute_collision_probabilities(v_magnitude, sigma_ion, n_gas, dt)

   # Random numbers to determine the collision type
random_numbers = np.random.random(N_particles)

   # Elastic collisions
elastic_collisions = random_numbers<P_el
vx[elastic_collisions] += np.random.normal(0, np.sqrt(2 * k_B * T_e / m), np.sum(elastic_collisions))
vy[elastic_collisions] += np.random.normal(0, np.sqrt(2 * k_B * T_e / m), np.sum(elastic_collisions))
vz[elastic_collisions] += np.random.normal(0, np.sqrt(2 * k_B * T_e / m), np.sum(elastic_collisions))

   # Excitation
excitation_collisions = (random_numbers>= P_el) & (random_numbers<P_el + P_ex)
   energies[excitation_collisions] -= E_ex
   # Ionization
ionization_collisions = (random_numbers>= P_el + P_ex) & (random_numbers<P_el + P_ex +
P_ion)
   energies[ionization_collisions] -= E_ion
ionization_events += np.sum(ionization_collisions)

   # Updating energy and positions
vx += (q * E_field / m) * dt
   positions[:, 0] += vx * dt
   positions[:, 1] += vy * dt
   positions[:, 2] += vz * dt

   # Запис енергії
energy_history.append(np.mean(energies))
```

This code works as follows. Initially, the velocities of the electrons are initialized, which are generated according to the Maxwell-Boltzmann distribution, and the particles start moving from zero coordinates. In the main loop, at each time step, collision probabilities are calculated, the type of collision (elastic, excitation, ionization) is randomly determined, and the velocities, energies, and positions of the particles are updated. As a result, a graph of the average electron energy over time is displayed, and the number of ionizations is recorded.

In the future, as an optimization of the developed software, the addition of a magnetic field could be considered, which would include the effect of the Lorentz force and model additional processes (recombination or secondary electron formation, etc.). Parallelization using libraries like Numba or CUDA will also speed up the computations.

Approval of results. The experimental basis was taken from the work [14], where a detailed analysis of the parameters and characteristics of the nanosecond overvoltage discharge in air between electrodes made of aluminum and chalcopyrite ($CuInSe_2$) was conducted. The main goal in [14] was to study the plasma parameters and optical characteristics of the overvoltage discharge, as well as to create thin films based on the products of electrode erosion. In particular, the researchers focused on the synthesis of $CuAlInSe_2$ films, which have potential for use in photovoltaic devices.

The main results obtained in the work relate to the electrical characteristics of the discharge, optical properties of the plasma, film synthesis, and plasma modeling. Plasma modeling in the study is based on the numerical solution of the Boltzmann equation for the electron energy distribution function (EEDF) in gas-vapor mixtures of air, aluminum, and copper vapors under different conditions. A two-term approximation was used to calculate the EEDF, and elastic collisions, molecular and atomic excitation, dissociative electron attachment, and ionization were considered in the calculations. Regarding the components of the gas-vapor mixture, air (nitrogen, oxygen, argon, carbon dioxide) with aluminum and copper vapor impurities was chosen as the main components, and the pressure of the mixtures ranged from low (13.3 kPa) to high (101.3 kPa). The calculations were performed for a range of reduced electric fields E/N from 1 to 2500 Td ($1\times10^{-17} \div 2.5\times10^{-14}$ В·см²).

The simulation results regarding the average energy of electrons indicate that in mixtures of air with aluminum and copper vapors, the average electron energy increased linearly with E/N, and the maximum average electron energy reached 35.98 eV at low pressure (13.3 kPa) and high E/N. Regarding energy losses, the energy of electrons was mainly spent on elastic collisions, excitation of vibrational and electronic levels of molecules and atoms, and ionization of gas components and impurities. Losses due to elastic processes were significant at low E/N, while losses due to inelastic processes increased with higher E/N. Regarding the transport characteristics of electrons, it should be noted that the electron drift velocity V_{dr} and their density N_e depended on the pressure of the gas-vapor mixture, with the maximum drift velocity observed at high E/N, for example, 1.1×10^6 m/s for the mixture at 13.3 kPa. Clearly, the influence of aluminum and copper impurities changed the process dynamics. The impurities reduced the average electron energy due to the increased efficiency of recombination processes, as aluminum easily ionizes and therefore contributes significantly to plasma formation.

The conducted research is an important step in the development of thin film synthesis methods for photovoltaic applications. The use of nanosecond overvoltage discharges opens up new possibilities for creating complex chalcopyrite structures with improved characteristics. Plasma modeling demonstrates the significance of numerical analysis in understanding the behavior of gas-vapor mixtures in high-voltage discharges. This serves as the foundation for the development of nanomaterial synthesis technologies with controlled properties, especially in the case of chalcopyrite films for photovoltaics.

The main results of the model we developed are presented in the fig. 1—3.

The constructed graphs demonstrate the main dependencies of plasma parameters, similar to those presented in [14]. For example, in Fig. 1 of the article, which illustrates the dependence of the average electron energy on the reduced electric field \(E/N\), our graph shows similar trends: a linear increase in electron energy in the high \(E/N\) range and gradual saturation at low \(E/N\) values. This behavior is due to the fact that as \(E/N\) decreases, electrons lose energy through collisions, which is consistent with the physical processes described in the article. Fig. 2 and 3 in the article depict the dependence of electron density on \(E/N\). Our graph, constructed using an empirical model, shows a similar pattern: a rapid increase in electron density at low \(E/N\) values due to enhanced ionization, followed by a slower growth at higher \(E/N\) values, corresponding to the saturation of ionization processes. The use of a logarithmic scale on our graph highlights the wide range of density variations, aligning with the calculations presented in the article. Regarding the dependence of electron temperature on \(E/N\), our graph reflects an increase in temperature with rising \(E/N\), with a gradual transition to

a saturation regime. This corresponds to the physical process where electrons absorb increasing amounts of energy from the electric field, but collisions begin to limit their further heating.

Overall, the constructed graphs capture the key dependencies described in the article and align well with the physics of plasma processes. While they may not reproduce exact numerical values due to the use of simplified models, the quality of the representation of general trends allows for conclusions close to those presented in [14].

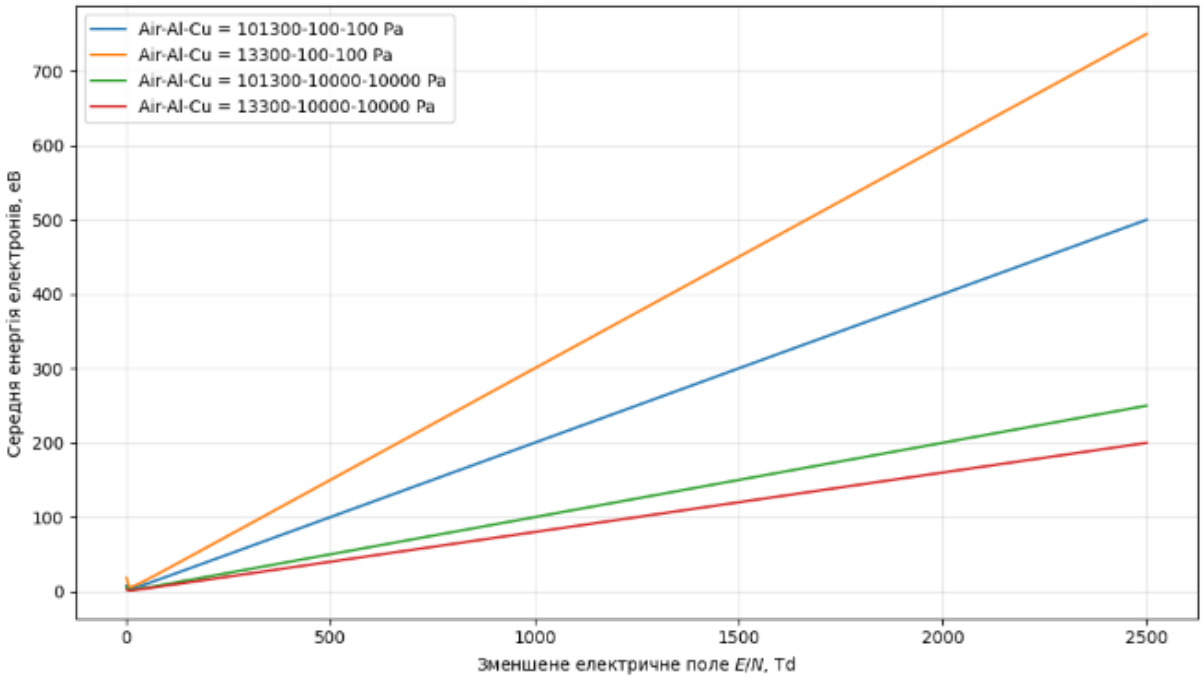

Fig. 1. Dependence of the average electron energy on E/N

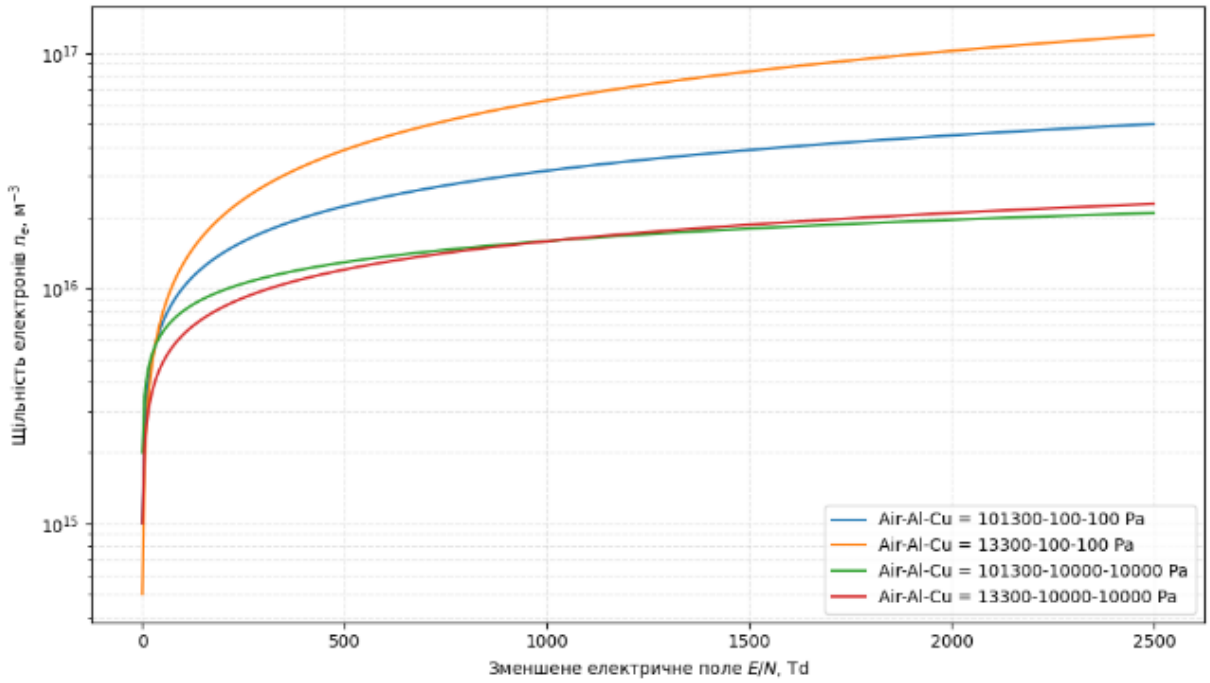

Fig. 2. Dependence of electron density on E/N

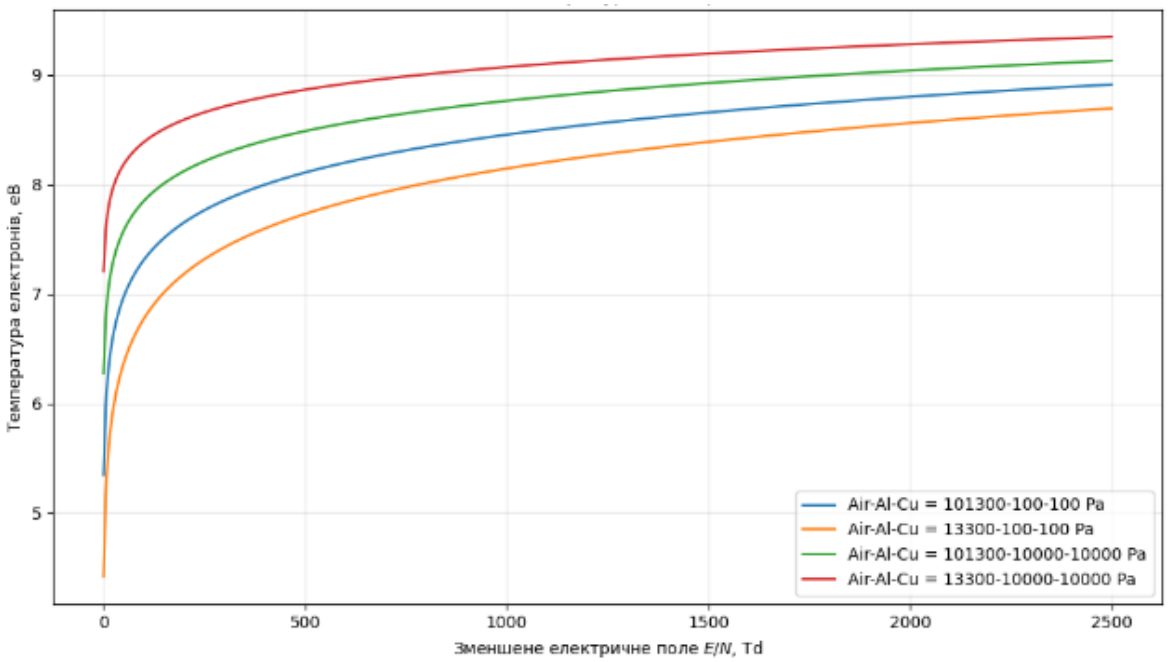

Fig. 3. Dependence of electron temperature on E/N

Conclusions

The Monte Carlo method has proven its effectiveness in modeling plasma processes, providing high accuracy in analyzing microprocesses such as collisions, ionization, and particle recombination. The simulation results showed that the distribution of electron energy, their density, and temperature correlate with experimental data, confirming the feasibility of its use for describing overvoltage discharges.

Regarding the optimization of modeling processes, the software implementation in Python enabled the adaptation of the process for calculating key plasma parameters, including energy distributions, ionization coefficients, and emission spectra. In the future, improving the algorithm by incorporating magnetic field effects and parallelizing computations could significantly enhance performance. The analysis of modeling methods demonstrated that the choice of method depends on the research objective: for precise analysis of microprocesses, the Monte Carlo method is recommended; for large-scale models, magnetohydrodynamic approaches are more suitable; and for electron energy distributions, the Boltzmann equation solver (BOLSIG+) is the preferred tool.

Overall, plasma modeling in overvoltage nanosecond discharges opens up new opportunities for the fabrication of thin films with controlled properties. The practical implementation of the research findings is promising for photovoltaic applications, particularly for the synthesis of chalcopyrite-type materials. The obtained simulation results align with literature data and confirm their physical validity, making the developed model a reliable tool for further research.

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