Numerical Simulation of Electrodynamic Structure of Penning Discharge in Large Volume Discharge Chamber with Annular Anode

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Abstract. In the study numerical simulation of electrodynamic structure of Penning gas discharge formed in large volume discharge chamber with annular anode is performed. For numerical modelling computer code implementing two dimensional axisymmetric electrostatic particle-in-cell method on unstructured grids is used. Computer simulation results of the Penning gas discharge in He under pressure $3 \times 10^{-4} - 9 \times 10^{-3}$ mbar, anode voltage 1-2 kV in the presence of external magnetic field $B \approx 0.1$ T are provided. Comparison of numerical and experimental results is performed.

1. Introduction

Typically, depending on application, Penning gas discharge plasma is formed ether in molecular hydrogen [1-3] or in helium [4, 5]. However, other buffer gases, such as neon or argon, are also used [6-8]. Molecular hydrogen is used in case when Penning ion source is part of the neutron generator [1-3]. Noble gases (helium, argon, neon) are used in case when plasma of Penning gas discharge is utilized as a light emitting source [4-8].

Most of numerical simulations are aimed at the investigation of spatial electrodynamic structure of Penning gas discharge in molecular hydrogen [9-14]. For the sake of development of numerical models of Penning gas discharge and validation of these models in this study results of numerical analysis using PIC-MCC method of large volume Penning gas discharge in helium experimentally studied in [4] are going to be presented.

Structure of the paper is as follows. In section 2 brief description of experiments reported in [4] will be given. In section 3 numerical model of considered Penning discharge based on PIC-MCC method will be described. In section 4 results of numerical analysis of selected experimental conditions are going to be presented.

2. Description of experiments

The study [4] is dedicated to the development of light emitting source, based on the large volume Penning discharge with single and double annular anodes. Schematic view of experimental setup is shown in figure 1. Developed discharge chamber consists of two cylindrical cathodes made of stainless steel. Radius of cathodes is 6 cm, distance between them is 5.5 cm. Cylindrical cathodes are connected to top and bottom flanges of vacuum chamber.
Two different configurations of gas discharge chambers were studied in [4]: with single annular anode and double annular anode (figures 2 and 3). In the first case anode ring with circular cross section radius 0.4 cm, inner diameter 6.45 cm and outer diameter 7.25 cm is placed at the height of 2.25 cm from the bottom cathode. In the second case two similar rings are located between cathodes. The distance between two rings is 2 cm. The bottom ring is placed at the height of 0.75 cm from the bottom cathode. Teflon rods are used in order to keep anodes in the given position.

![Figure 1. Schematic view of experimental setup developed in [4] (figure is borrowed from [4]).](image1)

Magnetic field is created by means of neodymium magnets placed behind the cathodes. Authors of [4] state that magnetic field is almost uniform and its induction is 0.1 T in the center.

The buffer gas is helium.

![Figure 2. Schematic view of discharge chamber in single anode configuration (figure is borrowed from [4]).](image2)

![Figure 3. Schematic view of discharge chamber in double anode configuration (figure is borrowed from [4]).](image3)

In [4] dependences of discharge current on applied anode voltage was measured in the wide range of buffer gas pressures for two anode configurations. Results of measurements are shown in figures 4 (single anode) and figure 5 (double anode).
Results of estimation of electron plasma density for single and double anode configurations at working gas pressure 9·10^{-4} mbar are presented in [4]: \( n_{e}^{sa} = 2\cdot10^{10} \text{ cm}^{-3} \), \( n_{e}^{da} = 2\cdot10^{11} \text{ cm}^{-3} \) correspondingly.

For the sake of numerical simulation it is necessary to estimate various plasma parameters relevant to the problem such as mean free path \( \lambda \), Debye length \( \lambda_{D} \), plasma frequency \( \omega_{p} \), cyclotron frequency and Larmor radius of electrons (\( \omega_{pe}, r_{le} \)) and ions (\( \omega_{pi}, r_{li} \)). Results for the single anode configuration are summarized in table 1.

![Figure 4](image1.png)  
**Figure 4.** Results of measurements of dependence of discharge current on anode voltage for single anode configuration (figure is borrowed from [4]).

![Figure 5](image2.png)  
**Figure 5.** Results of measurements of dependence of discharge current on anode voltage for double anode configuration (figure is borrowed from [4]).

| \( T_{e} \), eV | \( \lambda_{D} \), cm | \( \lambda \), cm | \( r_{le} \), cm | \( r_{li} \), cm | \( 1/\omega_{p} \), s | \( 1/\omega_{pe} \), s | \( 1/\omega_{pi} \), s |
|-----------------|---------------------|-----------------|-----------------|-----------------|----------------|----------------|----------------|
| 1               | 5.2\cdot10^{-3}     |                 |                 |                 |                |                |                |
| 5               | 1.2\cdot10^{-2}     | 1500            | 0.15            | 12.8            | 1.25\cdot10^{-10} | 5.7\cdot10^{-11} | 4.15\cdot10^{-7} |
| 10              | 1.6\cdot10^{-2}     |                 |                 |                 |                |                |                |

### Table 1. Results of estimation of various plasma parameters.

3. **Description of the model of Penning discharge in helium**

Numerical model of Penning gas discharge is based on 2D/3V axisymmetric electrostatic particle-in-cell – Monte-Carlo collision method. According to PIC-MCC method each time step macroparticles, which simulate behavior of large number of real plasma particles (electrons or ions) move in the self-consistent electromagnetic field and participate in collision processes. Each time step consists of several stages shown in the figure 6. Detailed description of numerical algorithms and methods at the core of computer implementation of each stage is described in [15, 16]. Here we are going to discuss only several topics connected with the modeling of elementary processes using Monte-Carlo collision technique in the framework of particle-in-cell method.
Figure 6. PIC-MCC computational cycle.

3.1. Monte-Carlo collision method
Monte-Carlo collision method as it used in particle-in-cell simulations generally can be described by the following formulas [17, 18]:

\[ \varepsilon_i = 0.5 m_i V_i^2 \]  \hspace{1cm} (1)
\[ \sigma_m(\varepsilon_i) = \sigma_1(\varepsilon_i) + \ldots + \sigma_N(\varepsilon_i) \] \hspace{1cm} (2)
\[ P_i = 1 - \exp\left(-\Delta V_i \sigma_m(\varepsilon_i) n_{tg}(\vec{x}_i)\right) \] \hspace{1cm} (3)

These steps can be described as following. For each particle in the simulation one determines kinetic energy \( \varepsilon_i \) (1) and total cross-section \( \sigma_m \) (2). In (2) only processes that are specific for given particle kind are considered. After that according to (3) one determines the probability of collision occurrence: if a random number uniformly distributed on the interval \([0,1]\) is less then \( P_i \) than collision occurs. In (3) \( V_i \) and \( \vec{x}_i \) are the velocity and position of the given particle correspondingly, \( n_{tg}(\vec{x}_i) \) is the local density of the target species at the position of the \( i \)-th particle and \( \Delta t \) is the time step. Let focus our attention on the last value.

One can choose a common time step for computation of particles motion and for computation of collision processes. However this might lead to the problems:

1. In case \( \Delta t \) is small the expression in the exponent can tend to zero as well as \( P_i \), which means that there will be no collision processes at all.

2. Monte-Carlo collision procedure is quite time consuming (even in the case of null-collision modification [18]). If one would compute it each time step it would significantly enlarge computational time needed for the problem to be solved.

Another choice is to set \( \Delta t \) independently on the time step for particles motion calculation. In this case one needs some criteria to impose on \( \Delta t \) in order to obtain valid results. The physical restriction which has to be applied to this value is that probability of more than one collision for given particle has to be negligible on the chosen time step. In [18] the probability of occurrence of more than one collision for the given particle was estimated:

\[ r \sim \sum_{k=2}^{\infty} P_i^k = \frac{P_i^2}{1 - P_i} < 0.01 \] \hspace{1cm} (4)

It yields \( P_i < 0.095 \) and \( \Delta V_i \sigma_m(\varepsilon_i) n_{tg}(\vec{x}_i) < 0.1 \).

3.2. Models of elementary processes
In the model of Penning discharge in helium two kinds of macroparticles are considered: electrons and helium ions. Two elementary processes are accounted for in the model of Penning discharge in helium:

1. \( \text{He} + e \rightarrow \text{He} + e \) (elastic scattering of electrons on atom \( \text{He} \));
2. $He + e \rightarrow He^+ + e + e$ (ionization of atom $He$ in collisions with electrons);

Cross-sections for these processes can be found in [19 - 21]. In [19] 1D kinetic simulation of direct current glow discharge in helium is performed. In the model following elementary processes for the helium plasma are included: elastic momentum transfer, full excitation, direct ionization, stepwise ionization, superelastic collisions and excitation of He atoms. In [20] cross-section database for excitation and ionization processes of helium atoms is presented. In [21] cross-sections for elastic scattering and ionization of He atoms was calculated based on the convergent close-coupling theory.

Cross-section for the elastic scattering of electrons on He atoms was taken from [21], cross-section for the ionization of He Atoms in collision with electrons was taken from [20]. In Figure 7 cross-section for both of these processes are shown.

As for the processes at the boundaries ion-electron emission from the cathode is accounted for in the model. The data on the dependence of the electron yield per ion versus energy was taken from [22].

![Cross-sections of the processes considered in the model.](image)

In the rest of this section the models of scattering and ionization processes [18, 23] that are used in order to create new particles in the simulation will be described.

Velocity of electron changes in direction and absolute value after elastic scattering on the neutral particle [18]. In order to account for the change in the direction two angles are computed: polar $\chi$ and azimuthal $\varphi$. Both angles are computed by means of random number uniformly distributed in the range [0,1]. Formula for azimuthal angle is:

$$\varphi = 2\pi R$$

Approximate expression for differential cross-section is used for calculation of polar angle [18]:

$$\cos \chi = \frac{2 + \varepsilon - 2(1 + \varepsilon)R}{\varepsilon}$$

here $\varepsilon$ is the initial kinetic energy of electron. Knowing both of these angles one can compute direction of the electron velocity after scattering. Corresponding expressions are presented in [18] and [22]. In [22] expressions for Cartesian components of velocity vector after scattering are given. In order to use formula from [18] one has to take into account that $\vec{i} = (1,0,0)$, $\cos \theta = \nu_\perp$ and
\[ \sin \theta = \sqrt{v_y^2 + v_z^2} \]. After algebraic manipulation it can be shown that formulas of [18] and [22] are coincident.

It is worth noting that high energy electrons scatter in the forward direction, while low energy electrons scatter isotropic.

In order to determine kinetic energy of the electron after scattering one can use the following formula [18, 24]:

\[ \frac{\Delta \varepsilon}{\varepsilon} = -\frac{2m}{M}(1 - \cos \chi) \]  

(7)

here \( m \) is the mass of electron and \( M \) is the mass of neutral particle. Using kinetic energy calculated according (7) one can fully define velocity of the scattered electron.

It is worth noting that particle-in-cell method used in the study is axisymmetric. It means that one has to transform electron velocity from cylindrical coordinate system to Cartesian before the application of the formulas presented above. Also conclusion step is to convert Cartesian velocity of scattered electron to cylindrical coordinate system.

Formulation of the model of ionization of neutral particles in the framework of PIC-MCC method starts with the energy conservation equation [18, 23]:

\[ E_{\text{scat}} + E_{\text{ej}} + E_{i} = E_{\text{inc}} + E_{\text{N}} - E_{\text{ion}} \]  

(8)

here \( E_{\text{scat}} \) is the energy of scattered electron, \( E_{\text{ej}} \), \( E_{i} \) is the energy of electron and ion created in the process of ionization, \( E_{\text{inc}} \) is the energy of incident electrons, \( E_{\text{N}} \) is the energy of neutral particle, \( E_{\text{ion}} \) is the ionization energy (ionization energy of He atom \( E_{\text{ion}} = 24.587 \text{ eV} \)). Let assume that in the process of ionization energy of created ion is no differ significantly in comparison with the energy of original neutral particle. In this case energy conservation equation becomes:

\[ E_{\text{scat}} + E_{\text{ej}} = E_{\text{inc}} - E_{\text{ion}} \]  

\[ E_{i} = E_{\text{N}} \]  

(9)

In this case one has to determine how the energy of incident electron divided between created electron and scattered electron. Formula for the calculation of the energy of created electron is given in [18, 23]:

\[ E_{\text{ej}} = B(E_{\text{inc}}) \tan \left[ R \arctan \left( \frac{E_{\text{inc}} - E_{\text{ion}}}{2B(E_{\text{inc}})} \right) \right] \]  

(10)

As energies of the scattered and ejected electrons are determined polar and azimuthal angles are calculated according to (5)+(6). Velocity of newly created ion is determined by means of Maxwell distribution and temperature of the neutral gas, which is the parameter of the model (for the results presented in the study \( T = 300 \text{ K} \)).

It is important to remind regarding the need of transformation of velocities from cylindrical to Cartesian coordinate system and backwards.

4. Numerical results of simulation of helium plasma of Penning discharge

In the section results of numerical simulation of helium plasma of Penning discharge will be presented. Numerical modeling was performed on the mesh presented in figure 8. Mesh consists of 4412 points and 8566 elements. Boundary conditions for Poisson equations are:

\[ \frac{\partial \phi}{\partial r} \bigg|_{r=0} = 0; \quad \phi \bigg|_{r=6} = \phi \bigg|_{r=-6} = \phi \bigg|_{z=5.5} = 0 \]  

\[ \phi \bigg|_{\text{anode boundary}} = V_a \]  

Anode is located in the center of computational domain (white box in the figure 8), \( V_a \) is anode voltage.
All presented results are obtained using the assumption that magnetic field inside the discharge chamber is not uniform. The distributions of radial $B_r$ and axial $B_z$ components of induction of magnetic field are presented in figures 9 and 10. Magnetic field was calculated according to method described in [25].

Initially two electrically neutral clouds were distributed in the computational area. The first one is located above anode and the second one is located below anode. Each cloud consists of 120000 electrons and 120000 ions He$^+$. Weight of the particles in the cloud varies ($\sim 7 \cdot 10^5 \div 4 \cdot 10^6$) depending on the simulation in order to maintain reasonable amount of particles in the computational domain. Initial velocities of the macroparticles were sampled using Maxwell distribution at temperature 300 K. For the carried out numerical simulations time step is $5 \cdot 10^{-12}$ s.

Numerical modeling of the helium plasma of Penning discharge was conducted at following parameters:
1. p = 9·10^{-4} mbar (0.675 mTorr), V_a = 2000 V;
2. p = 9·10^{-4} mbar (0.675 mTorr), V_a = 1000 V;
3. p = 3·10^{-4} mbar (0.224 mTorr), V_a = 2000 V;
4. p = 3·10^{-4} mbar (0.224 mTorr), V_a = 1000 V.

In figure 11 spatial distribution of the electric potential \( \phi \) [V] is presented for the first set of conditions. Spatial distributions of axial \( E_z \) [V/cm] and radial \( E_r \) [V/cm] components of electric field are presented in figure 12. One can notice bending of the distributions with edges directed towards the axis of symmetry. This effect is due to nonuniform magnetic field. Numerical experiments conducted at uniform magnetic field with \( B_z \neq 0 \) and \( B_r = 0 \) yield distributions without such bending.
In figure 13 and 14 distributions of the electric potential and radial component of electric field along the line $z = 2.75$ cm (line perpendicular to the axis symmetry and passing through its center) are given for 4 sets of parameters considered in the study. Anode is located in these figures in the range of $r \in [3.25; 3.65]$ cm.

**Figure 13.** Distribution of the electric potential along line $z = 2.75$ cm (from $r = 0$ cm–axis of symmetry to $r = 6$ cm) for different conditions.

**Figure 14.** Distribution of the radial component of electric field along line $z = 2.75$ cm (from $r = 0$ cm–axis of symmetry to $r = 6$ cm) for different conditions.
One can notice that anode layers exists in the discharge. Also one can notice presence of local maxima around 100-200 V in the center of the discharge chamber.

In figure 15 and 16 spatial distribution of number density of electrons and He\(^+\) ions in computational area is shown for \(p = 9 \cdot 10^{-4} \text{ mbar} , V_a = 2000 \text{ V}\).

**Figure 15.** Spatial distribution of electrons number density \(n_e \left[ \text{cm}^{-3} \right]\) at \(p = 9 \cdot 10^{-4} \text{ mbar} , V_a = 2000 \text{ V}\).

**Figure 16.** Spatial distribution of He\(^+\) ions number density \(n_i \left[ \text{cm}^{-3} \right]\) at \(p = 9 \cdot 10^{-4} \text{ mbar} , V_a = 2000 \text{ V}\).
In figure 17 distributions of the number density of electrons and He$^+$ ions along the line $z = 2.75$ cm (line perpendicular to the axis symmetry and passing through its center) are shown for the same conditions.

![Graph showing distributions of electron and He$^+$ ion number density along line $z = 2.75$ cm](image)

**Figure 17.** Distribution of the electrons and H$_2^+$ ions number density along line $z = 2.75$ cm (from $r = 0$ cm– axis of symmetry to $r = 6$ cm) at $p = 9 \cdot 10^{-4}$ mbar, $V_a = 2000$ V.

It can be seen from figures that number density of electrons reaches it maximum in the vicinity of anode. The maximum is about $1.5 \cdot 10^{10}$ cm$^{-3}$ which agrees with estimation given in [4]. There is the offset about 0.4 cm between maximums in number densities of electrons and ions in the vicinity of anode. As can be seen from figure 15 - 17 there is a region of almost quasineutral plasma in the central part of computational domain ($r \in [0.2; 2.4]$ and $z \in [2.4; 3.2]$).

Plots on figures 18 and 19 allow estimating variation of number density of electrons and ions in dependence on the discharge parameters. In the figure 18 and 19 distribution of the number density of electrons and He$^+$ ions along the line $z = 2.75$ cm are shown for the 4 sets of discharge conditions. One can notice that generally maximum of electron density for all sets of conditions is located near anode. Maximum of $n_e$ decreases with decreasing pressure and anode voltage. One can notice presence of the second local maximum of electrons near the axis of symmetry except for the case $p = 3 \cdot 10^{-3}$ mbar, $V_a = 1000$ V. Maximum of $n_i$ for all conditions is located near the axis of symmetry. Maximum of $n_i$ decreases with decreasing anode voltage and pressure as well as the maximum of $n_e$. Second local maximum of He$^+$ ions near the anode clearly distinct at conditions corresponding to the anode voltage $V_a = 2000$ V. Regions of quasineutral plasma are observed for all condition sets considered in the study. However the largest quasineutral region exists at $p = 9 \cdot 10^{-4}$ mbar, $V_a = 2000$ V.

In figures 20 ÷ 22 distributions of electron and He$^+$ ion temperatures are presented for the first condition set. Maximums of electron temperature are located in the vicinity of anode and reach 130 eV. In the bulk of plasma electron temperature is 10 eV. Maximums of ion temperature are located in the vicinity of local maximum of ions number density near $r \in [2.6; 2.8]$ and reach 400 eV.
Noticeable that temperature of ions reaches local minimum ~150 eV in the region of local ion density maximum.

![Figure 18](image1.png)

**Figure 18.** Distribution of electron number density along line $z = 2.75$ cm (from $r = 0$ cm– axis of symmetry to $r = 6$ cm) for different conditions.

![Figure 19](image2.png)

**Figure 19.** Distribution of He$^+$ ions number density along line $z = 2.75$ cm (from $r = 0$ cm– axis of symmetry to $r = 6$ cm) for different conditions.
Figure 20. Spatial distribution of electron temperature $T_e$ [eV] at $p = 9 \cdot 10^{-4}$ mbar, $V_a = 2000$ V.

Figure 21. Spatial distribution of He$^+$ ions temperature $T_i$ [eV] at $p = 9 \cdot 10^{-4}$ mbar, $V_a = 2000$ V.
In figures 23 and 24 distribution of the electrons and He\(^+\) ions temperatures along the line \(z=2.75\) cm are shown for the 4 sets of considered discharge conditions. For all conditions temperature of electrons reaches two maxima on both sides of anode. Temperature of the electrons in these maxima decreases at decreasing anode voltage from 85 to 40 eV. Temperature of electrons in the bulk of plasma is \(~10\) eV for all considered conditions. As for the ion temperature it is noticeable that two maxima in \(T_i\) vanish as local (in the vicinity of the anode, see figure 19) ion number density vanish.

In the figure 25 energy distribution functions of electrons and ions for different discharge parameters are presented. It can be seen that energy distribution functions mostly varies with the anode voltage. Dependence on the discharge pressure is not prominent. Electron energy distribution functions can be approximated using two temperature distributions. According to the results of numerical simulation one can observe that energy distribution function of ions resembles plateau in the range 1000\(-\)1700 eV for cases where anode voltage \(V_a = 2000\) V and in the range 250\(-\)750 eV for cases where anode voltage \(V_a = 1000\) V.

In the figure 26 comparisons of experimental and numerical data is presented. Blue symbols are results of numerical simulation, black symbols and lines are experimental data. It can be seen that at higher pressures agreement of numerical and experimental data is satisfactory. At low pressures discrepancy is high. Nevertheless presented numerical model of Penning gas discharge in helium correctly describes trend in changing of the discharge current, i.e. discharge current increases at increasing pressure and anode voltage. If one sums steady state current through anode and cathode (considering sign of the current) than the resulting value would oscillate near zero. The maximum deviation of the value varies in the range 14\(-\)30\% of discharge current shown in figure 26.
Figure 23. Distribution of electron temperature along line $z = 2.75$ cm (from $r = 0$ cm– axis of symmetry to $r = 6$ cm) for different conditions.

Figure 24. Distribution of He$^+$ ions temperature along line $z = 2.75$ cm (from $r = 0$ cm– axis of symmetry to $r = 6$ cm) for different conditions.
**Figure 25.** Energy distribution functions of electrons and ions for different discharge parameters.

**Figure 26.** Comparison of experimental and numerical data.
5. Conclusion
In the study numerical model of Penning gas discharge in helium was described. Model was applied for the simulation of electrodynamic structure of helium plasma of large volume Penning discharge at experimentally investigated parameters. Electrodynamic structure of the Penning gas discharge in helium at pressure $p=3\cdot10^{-4} \div 9\cdot10^{-4}$ mbar and anode voltage $V=1000\div2000$ V was obtained and analyzed. Distribution of potential, electric field, charged particles number densities, temperatures and energy distribution functions are presented. Results of simulation are compared with the experimental data for the validation of numerical model.

Presented numerical model of Penning gas discharge in helium correctly describes trend in changing of the discharge current. Agreement of numerically predicted and experimental discharge current is acceptable, while at low pressure discrepancy is significant.

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