Validation of Numerical Model of Penning Gas Discharge based on 2D/3V PIC-MCC Method

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Abstract. The data obtained in the experiments conducted in University of California, Berkley are used to validate numerical model of Penning gas discharge. Numerical model is based on 2D/3V axisymmetric electrostatic particle-in-cell method implemented on unstructured grids. Elementary processes in the gas discharge plasma are simulated using Monte-Carlo collision method. Electrodynamic structure of the Penning gas discharge is obtained using mentioned numerical model under conditions relevant to experimental and analyzed. Distributions of the potential, electric field, electrons and ions number densities, temperatures, distribution functions are presented in the study. Validation of numerical model is performed by comparison of the dependence of discharge current on applied magnetic field.

1. Introduction
The plasma of Penning gas discharge is stable at relatively low pressure. This effect is achieved by placing plasma in quadrupole electric field and axial magnetic field. Electrons are trapped within these fields and produce substantial ionization in order the plasma to be selfsustained. Due to the fact that Penning gas discharge exists at low pressure, PIC-MCC method \cite{1,2} is a good approach for simulation of the considered physical system.

2D/3V axisymmetric electrostatic PIC-MCC method suitable for simulation of electrodynamic structure of the Penning gas discharge was implemented and analyzed in \cite{3,4}. Verification of the solver was performed on the basis of 2D Child-Langmuir problem. Results of verification were reported in \cite{3}. In the present study numerical experiments were conducted in order to validate numerical method against available experimental data.

In the past ten years several studies has been performed dedicated to the experimental investigation of the Penning gas discharge \cite{5–11}, however not all of them is possible to use for the validation purposes. Kreindel and Ionov \cite{5} conducted experiments with annular anode. They were able to record the dependence of discharge and extracted current on the magnetic field. Due to the usage of annular anode it was possible to make a photo of the discharge. However in the original study \cite{5} several parameters (diameter of the annular anode and type of the gas) are missing which make impossible to use this work for the validation purposes.

In \cite{6} volt-ampere characteristics of the Penning gas discharge in molecular hydrogen were obtained for the various geometric parameters of discharge chamber and H\textsubscript{2} pressure. Much data were gathered and presented in \cite{6} however usage of anodes (“long” and “short”) and anticathode made of
wire mesh as well as annular magnets introduce uncertainties in the process of analysis of the discussed experimental results.

The studies [7, 8] were dedicated to the development of the compact Penning discharge chamber suitable for the usage as the ion source. Experimental investigation of the proposed design of the Penning discharge chamber was conducted for various gasses (molecular hydrogen, helium) in the wide range of pressures and anode voltages. Geometry of the proposed discharge chamber is given in details however lack of information regarding the permanent cylindrical magnet and substantial inhomogeneity of the magnetic field in the system does not allow using this work directly for the validation of the developed solver.

In the studies [9, 10] spectral radiation of the large volume Penning gas discharge in helium was investigated. Ring and double-ring anode configuration were considered. Parameters of the conducted experiments are given in details. For the purposes of validation of the computer code volt-ampere characteristics measured in the wide range of gas pressure can be used. However use of annular anode implies difficulties in the formulation of the boundary conditions in the process of numerical simulation.

In [11] classical Penning gas discharge has been studied. Cylindrical anode is placed between two circular cathodes with small gaps (relative to the size of anode) between cathode and anode. Experimental parameters relevant for the numerical simulation are given the study. External magnetic field is produced by electric coil. For the validation of the PIC-MCC solver dependence of the discharge current on the magnetic field is given in [11].

In the study analysis of electrodynamic structure of the Penning gas discharge relevant for the conditions of the experiments presented in [11] is performed. Distribution of potential, electric field, electrons and ions number densities, temperatures and distribution functions are given. Validation of the numerical model is performed by calculating dependence of the discharge current on the magnetic field and comparing it against available experimental data.

2. Brief description of the numerical model of Penning gas discharge

Particle-in-cell method introduces a concept of macroparticle [1, 2]. Macroparticle is a computational particle that simulates behaviour of a large number of real plasma particles (electrons or ions). Macroparticles follow the trajectory of real particles in the plasma since the Lorentz force depends only on the charge-to-mass ratio [12]. The movement of macroparticles changes the distribution of electromagnetic field in the system. It means that the whole simulation process is self-consistent. It can be shown that actually PIC method is a mean for solution of Vlasov-Maxwell system of equations [13].

For the numerical solution of the Penning gas discharge problem numerical model based on 2D/3V axisymmetric electrostatic PIC–MCC method was used. In order to briefly characterize numerical methods and approaches that have been used in the computer implementation of the PIC-MCC method mentioned above let us consider a computational cycle shown in figure 1.

The first stage of a computational cycle is the solution of the Poisson equation. It is formulated for the axisymmetric geometry:

$$\Delta \phi = \frac{1}{r} \left( \frac{\partial}{\partial r} \left( r \frac{\partial \phi}{\partial r} \right) + \frac{\partial}{\partial z} \left( r \frac{\partial \phi}{\partial z} \right) \right) = \frac{\rho(r,z)}{\varepsilon_0}$$  \hspace{1cm} (1)

In equation (1) $\phi$ is the electrostatic potential, $\rho(r,z)$ is the charge density and $\varepsilon_0$ is the electric constant. For the boundary value problem the boundary conditions can be formulated in the following form:

$$\left. \left( \alpha_1 \phi + \alpha_2 \frac{\partial \phi}{\partial n} \right) \right|_{\partial D} = g(r, z)$$  \hspace{1cm} (2)
For the numerical solution of equation (1) the computational domain is subdivided into triangles. Usage of unstructured grids for the numerical simulation of gas discharges is necessary since discharge chamber may be of complex shape. Descritization of equation (1) is carried out using cell-centered finite volume method [14]. The descritization process leads to a problem of calculation of potential derivative along the edge of the triangle [3]. For this purpose the least square method was used.

![Figure 1. PIC-MCC computational cycle.](image1)

The corresponding template consists of all triangles that contain at least one point of the considered edge (figure 2). Geometrical multigrid method is used for the numerical solution of the system of linear algebraic equations resulted from the descritization process. Implementation of the multigrid procedure on the unstructured grid is performed using overset meshes approach [15]. Obtained potential distribution as the solution of the Poisson equation is used for the calculation of the electric field within the computational domain. This process is performed in two stages. At the first stage least square method and template shown in figure 3 are used in order to calculate the electric field in the cell centers. At the second stage values of electric field in the cell centers are interpolated to the vertices of the mesh [16, 17].

![Figure 2. Template for calculation of potential derivative along the edge F₁F₂.](image2)
Figure 3. Template for the calculation of electric field in the cell centers.

Development of the particle-in-cell method on the unstructured grids requires special procedures of interpolation of the electric field to the particles position for the Lorentz force calculation and localization of macroparticles relative to the mesh elements (particle search algorithm) [13, 18]. These procedures constitute the second stage of the computational cycle. Both of these procedures can be easily implemented using local basis functions $N^k_n(z, r)$ constructed for the $n$-th node (local numbering of triangle nodes, varies from 1 to 3) of the $k$-th element (figure 4).

For the interpolation procedure the following property of the local basis function is important. If the values of interpolated function $f$ are known in the $k$-th triangle nodes $(z^k_m, r^k_m)$, then for every point with coordinates $(z_j, r_j)$ that lies inside triangle:

$$f(z_j, r_j) = \sum_{n=1}^{3} N^k_n(z_j, r_j) f(z^k_n, r^k_n)$$

(3)

For the macroparticle search algorithm the following property is used [13, 18]. If the macroparticle lies within the $k$-th triangle then the values of all local basis functions $N^k_n(z_p, r_p)$ are nonnegative, where $z_p$ and $r_p$ are the axial and radial coordinates of the considered macroparticle.
In the third stage of the computational cycle one has to solve equations of particles motion. In the study only nonrelativistic case is considered. The resulting system of equations for the case of cylindrical coordinate system has singularity when particle with nonzero angular momentum approaches to the axis of symmetry [19]. If one is going to solve numerically this system it has to deal with the problem. Boris [12, 19] has proposed the numerical procedure which successfully overcomes mentioned above difficulty using Cartesian–cylindrical coordinate systems transformation.

Another problem is concerned with the Boris numerical method itself. Boris method is of the class of leap-frog methods, which means that velocities of the particles and their coordinates are not known in the same moments of time, however initial conditions are formulated in the same moment of time. In order to initialize calculation procedure correctly one has to obtain appropriate velocity of the particle. This problem was formulated and solved in [19].

On the next stage of computational cycle processes at the boundaries have to be considered. For example, plasma particles hitting the metal electrodes generate electric current. Dielectric boundaries are able to accumulate charge of plasma particles and impact on the distribution of the potential inside the discharge chamber [20]. Ions and electrons of plasma can hit surfaces of discharge chamber and generate fluxes of charge particles directed back to the gas discharge plasma due to the processes of secondary electron emission, ion-electron emission [21].

Accounting for the secondary emission processes at the boundaries can be implemented according to method described in [20]. Number of particles injected from the boundary into the computational area due to boundary-macroparticle collision is determined using the random number $R$ uniformly distributed on the interval $[0,1]$. If $R < (\gamma - \text{int}(\gamma))$ then number of particles to be injected into the computational area is $N_{\text{inj}} = \text{int}(\gamma) + 1$ otherwise $N_{\text{inj}} = \text{int}(\gamma)$. A model of the corresponding process has to be applied for the initialization of the new particles.

It is possible to account for elementary processes in the PIC algorithm using the Monte-Carlo collision approach based on the null collision method [22-24]. Monte-Carlo collision method consists of the following steps [23]. Calculation of the kinetic energy of the particle $i$ of sort $s$:

$$
\epsilon_i = 0.5m_iV_i^2
$$

Determining the magnitude of the total collision cross-section corresponding to this energy:

$$
\sigma_{\text{tot}}(\epsilon_i) = \sigma_s(\epsilon_i) + ... + \sigma_s(\epsilon_i)
$$

Here $\sigma_j(\epsilon_i)$ for $1 \leq j \leq N$ is the cross section of the $j$-th type of collision between the species $s$ and the target species. The collision probability is calculated using the following formula:

$$
P_i = 1 - \exp(-\Delta t V_i \sigma_{\text{tot}}(\epsilon_i)n_{xy}(\vec{x}_i))
$$

In (6) $V_i$ and $\vec{x}_i$ are the velocity and position of the $i$-th particle correspondingly, $n_{xy}(\vec{x}_i)$ is the local density of the target species at the position of the $i$-th particle. A collision occur if a random number uniformly distributed on the interval $[0,1]$ is less then $P_i$. If the collision occurs then one has to determine the collision type using another random number. After that new particles have to be initialized based on the model [22-25] of the process corresponding to the given collision type.

Disadvantage of the approach presented above is due to the necessity of calculation of $P_i$ for each particle in the simulation. In order to overcome this difficulty the null collision method was proposed. Detailed description of the method is given in [24]. The idea of the method is to introduce the constant collision frequency $\nu$ in the following manner:

$$
\nu = \max_{s,k} \left( n_{\text{des}}(\epsilon_i) \sigma_{\text{tot}}(\epsilon_i) \right) = \max_s \left( n_{\text{des}}(\epsilon_i) \right) \max_k \left( \sigma_{\text{tot}}(\epsilon_i) \right)
$$
Physically it means that additional collisional process is introduced with collision frequency of the special form. This collisional process is called null collision since no real interaction occurs. Then one can determine maximum fraction of the total number of particles of sort $s$ which experience collision:

$$P_{null} = 1 - \exp(-\nu'\Delta t)$$  \hspace{1cm} (8)

The colliding particles are chosen randomly among all the particles of the given sort $s$ participating in the simulation (eliminating duplicates), and each particle is checked for the type of the collision.

The last stage of computational cycle is the calculation of the charge density of plasma particles. These fields are used for the construction of source term for the Poisson equation. In case of unstructured grid and cylindrical coordinate system one can utilize the formalism of local basis function [13, 18] in order to perform the calculations. The corresponding formula can be written as follows [13]:

$$q_n = \frac{1}{V_n} \sum_k \sum_j Q_j N_n^k(z_j, r_j) \frac{1}{2\pi r_j}$$  \hspace{1cm} (9)

In (9) summation is performed over all particles $j$ that are in triangle $k$ that contains the node $n$. $z_j$ and $r_j$ are the axial and radial coordinates of macroparticle, $Q_j$ is the charge of macroparticle, in the two-dimensional case $V_n$ is calculated according to the following formula:

$$V_n = \sum_k \frac{S_k}{3}$$  \hspace{1cm} (10)

In (10) $S_k$ is the area of the triangle $k$ that contains node $n$.

3. **Problem formulation for simulation of experiments [11]**

Validation of the numerical model is performed on the basis of experiments, conducted in University of California, Berkley [11]. In the figure 5 schematic view of experimental setup is shown.

*Figure 5. Schematic view of the experimental setup (figure is taken from [11]).*
Cylindrical anode (A) with the length of 2.54 cm and diameter of 2.54 cm is placed inside the metallic chamber and isolated from it with insulator (D). There are two circular cathodes (B1, B2) on the both sides of anode. Cathodes are electrically isolated from the anode. Diameter of cathodes is 2.54 cm. The cathode B2 contains extraction orifice. Diameter of the extraction orifice is 0.2 cm. Electrodes of the discharge chamber are made of aluminium. External magnetic field in the system is created by an electromagnetic coil. This allowed varying the magnetic induction in the range 0.02÷0.05 T. In the experiments molecular hydrogen was used. The pressure of the gas was varied in the range 0.8÷1.0 mTorr. Anode potential was changed in the range 600÷800 V. In the experiments [11] dependence of the discharge current on the magnetic induction was measured (figure 6).

![Figure 6. Experimental measurement of the dependence of the discharge current on the axial magnetic field (figure is borrowed from [11]).](image)

Analysis of the described experiments was performed using the mesh presented in figure 7. Unstructured computational mesh consists of 2648 nodes and 5099 triangles. Computational mesh is uniform (no thickening). The boundaries of the computational domain coincide with the corresponding electrodes (see figure 5). Numerical simulation was performed at the anode voltage 800 V (cathodes are grounded), molecular hydrogen pressure 0.8 mTorr. Magnetic induction varied in the range 0.02÷0.033 T. For the numerical simulation time step is $4 \cdot 10^{-12}$ s.

Two kinds of macroparticles were taken into account: electrons and $H_2^+$ ions. At the beginning of the numerical simulation 120000 electrons and 120000 $H_2^+$ ions were placed in the cylindrical region of diameter of 1 cm and length of 1 cm in the center of computational area. Initial number density of charged particles is $1.5 \cdot 10^9$ cm$^{-3}$. Initial velocities of the macroparticles were sampled using Maxwell distribution at temperature 300 K.

Elementary processes accounted for in the study are elastic electron scattering on H$_2$ molecules ($e$+H$_2$→$e$+H$_2$) and ionization of H$_2$ molecules by electrons ($e$+H$_2$→H$_2^+$+$e$+$e$). The data on the cross-section for these processes were taken from [26]. Also ion-electron emission from the cathode has been taken into account. The data on the dependence of the electron yield per ion versus energy was taken from [27].

In the following section results of the validation of the numerical model presented above on the basis of the experiments described in [11] for various magnetic induction are going to be presented and analyzed.
4. Numerical results of Penning gas discharge simulation

Results of numerical simulation of Penning gas discharge at conditions relevant to experiments [11] are presented in this section. In details we will show and analyze results obtained at $B_z = 0.033$ T.

In the figure 8 temporal evolution of number of macroparticles in computational area is presented. The plot indicates that plasma tends to stationary state. Number of macroelectrons in stationary state is about 1.16 millions, number of macroions in stationary state is about $7 \cdot 10^5$. Weight of each macroparticle is about 40000.

In the figures 9–12 distribution of the potential $\phi$ [V] and $E_r$ [V/cm], $E_z$ [V/cm] components of electric field in the stationary state are presented. In the figure 9 direction (length of the arrow does not reflect absolute value of the electric field) of the electric field is indicated with black arrows. It is easy to observe that the potential reaches minimum (~50 V) in the region $r \approx 0.45$ cm. In this region electric field has only its $z$–component (figure 9). Potential rises to the anode which is obvious, however one can observe rise of the potential near the axis of symmetry (up to ~116 V).

$E_z$ component of the electric field is equal ~10 V/cm in the region of the Penning gas discharge existence (center of the computational area, figure 10). The maximum absolute value of the $E_z$ component of the electric field is about 4 kV/cm. This maximum value is reached near the edges of anode.

$E_r$ component of the electric field reaches the local maximum (~500 V/cm) in the region $r \approx 0.10$ cm. The maximum absolute value of the $E_r$ is reached near the anode and its edges.
Figure 8. Temporal behaviour of number of macroparticles in the system, $B_z = 0.033$ T.

Figure 9. Spatial distribution of potential $\varphi$ [V] in steady state, $B_z = 0.033$ T.

In figures 13–15 distribution of number densities of electrons and $\text{H}_2^+$ ions in the computational area is presented. The distribution of electrons in computational area reaches the maximum near the axis of symmetry and then falls to the anode. Near the region $r \approx 1$ cm one can observe the second local maximum in the distribution of the electron number density. The distribution of $\text{H}_2^+$ ions number density is similar to that of the electrons. The ions number density reaches the maximum near the axis of symmetry and then it falls down to the anode. The position of the global maximum in electrons and ions number density distributions are coincide. In the region $r = 0.15 - 0.6$ cm the number densities of electrons and ions coincide, which makes the plasma in that region quasineutral.
Figure 10. Spatial distribution of $E_z$ [V/cm] component of electric field in steady state, $B_z=0.033$ T.

Figure 11. Spatial distribution of $E_r$ [V/cm] component of electric field in steady state, $B_z=0.033$ T.

In figures 16–18 distribution of the electrons and $H_2^+$ ions temperatures in eV is presented. The temperatures of charged particles were calculated according to the following formula:

$$T(\vec{r},t) = \frac{m}{3n} \int f(\vec{r},\vec{v},t) (\vec{v} - \vec{u})^2 \, d\vec{v}$$

There are two local maxima in the distribution of $T_e$. The first one is near the axis of symmetry, the second one is close to anode. The temperature of the electrons in the maximum reaches $\sim 35$ eV. The distribution of ions temperature has plateau in the region $r \sim 0.2-0.8$ cm. The temperature of ions in this region is about 150–160 eV. The temperature of electrons in this region is $\sim 10-20$ eV. Using presented data on the charged particles number densities and temperatures one can estimate Debye radius and plasma frequency in the system. Based on the corresponding maximum values: $\omega_p \sim 8 \times 10^9$ s$^{-1}$ and $\lambda_D \sim 0.03$ cm.

In the figure 19 energy distribution function (EDF) of charged particles is presented. The EDF can be calculated according to the following formula:

$$f(\varepsilon) = \frac{dN}{Nd\varepsilon}$$
Figure 12. Distribution of the potential and component of electric field along line \(z=1.5\) cm (from \(r=0\) cm– axis of symmetry to \(r=1.27\) cm - anode) in steady state, \(B_z=0.033\) T.

Figure 13. Spatial distribution of electrons number density \(n_e\) [cm\(^{-3}\)] in steady state, \(B_z=0.033\) T. One can see that the maximum energy of charged particles do not exceed 800 eV, which correspond to the applied anode voltage. One can see that the EDF of both charged species is deviate from the Maxwell distribution (in opposite case the EDF would be linear). The tail of electrons and ions EDF is overpopulated as compared to Maxwell distribution. In the EDF of ions one can observe behavior that is close to plateau in the region 200÷600 eV.
Figure 14. Spatial distribution of H$_2^+$ ions number density $n_i$ [cm$^{-3}$] in steady state, $B_z=0.033$ T.

Figure 15. Distribution of the electrons and H$_2^+$ ions number density along line $z=1.5$ cm (from $r=0$ cm– axis of symmetry to $r=1.27$ cm - anode) in steady state, $B_z=0.033$ T.

In the figure 20 one can see the distribution of the ionization events versus energy of electrons. One can see that most electrons that participate in ionizing collisions have energies $\sim$46.5 eV. Also according to the simulation it was found that most electrons that emerged in the process of ion-electron emission from the cathode acquire energy of 100 eV in approximately 1 ns. According to the
numerical results most of the ions has lifetime $\sim 10^{-7}$ s. For the electrons similar distributions shows two peaks at values of lifetime $\sim 10^{-6}$ s and $10^{-10}$ s. However mentioned values are preliminary and require conduction of additional numerical experiments.

**Figure 16.** Spatial distribution of electron temperature $T_e$ [eV] in steady state, $B_x=0.033$ T.

**Figure 17.** Spatial distribution of $H_2^+$ ions temperature $T_i$ [eV] in steady state, $B_x=0.033$ T.

In figure 21 one can see comparison between experimental and numerical data. Dependence of the discharge current versus applied external magnetic field is shown. One can see reasonable agreement between measured and calculated data. However one can see (figure 6) that behavior of the current with increasing magnetic field is nonmonotonic. There exists $I_{\text{max}}$ and corresponding $B_{\text{max}}$ after which further increase in B leads to decrease in I. It is worth noting that similar behavior of the discharged current was observed in the experiments presented in [5] which might indicate that this is general behavior (not some feature of the considered experimental data) of current in dependence of the magnetic field. Further numerical investigation required in order to understand mentioned phenomena and check if the current version of the model is able to reproduce it.

Mass spectrum of the extracted current from the Penning ion source was measured in the experiments [11]. This measurement has shown the presence of hydrogen atoms in the extracted current. Validation of the model in that aspect is possible by introducing corresponding elementary
processes into it. In order to obtain estimate of the significance of the elementary processes that lead to the formation of hydrogen atoms studies [28-30] can be used.

**Figure 18.** Distribution of the electrons and H$_2^+$ ions temperature along line $z=1.5$ cm (from $r = 0$ cm– axis of symmetry to $r = 1.27$ cm - anode) in steady state, $B_z=0.033$ T.

**Figure 19.** Energy distribution function of electrons and ions in steady state, $B_z=0.033$ T.
Figure 20. Distribution of ionization events versus energy of electrons, $B_z=0.033$ T.

Figure 21. Comparison of experimental and numerical data.
Alternative method for the simulation of Penning gas discharge is modified drift-diffusion approach [31–34]. It seems that this model if properly set up might be used for the simulation of the Penning gas discharge.

5. Conclusion
In the study numerical model for the simulation of Penning gas discharge is applied for the analysis of experiments conducted in the University of California, Berkley. Electrodynamic structure of the Penning gas discharge at pressure p = 0.8 Torr, V = 800 V and B = 0.02–0.033 T were obtained and analyzed. Distribution of potential, electric field, charged particles number densities, temperatures and energy distribution functions are presented.

Results of modelling are compared with the experimental data for the validation of numerical model. Dependences of the discharge current on the applied external magnetic field obtained experimentally and numerically are in reasonable agreement.

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