Numerical Simulation of Penning Gas Discharge in 2D/3D Setting

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Abstract. This work presents a numerical simulation of the Penning discharge in 2D/3D formulation. The simulation is based on the electrostatic particle method in cells using structured rectangular grids and implemented in the VSim software package. To simulate the kinetic processes in a gas-discharge plasma, the Monte-Carlo collision method was used. The calculations were carried out for several sets of chemical kinetics reactions, and their comparison is given. Various characteristics of the Penning discharge in 2D and 3D formulation were calculated, such as anodic/cathodic currents, the distribution of charged particles in space and energies, etc. A comparison of the simulation results with experimental data was observed.

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 self sustained. Due to the fact that Penning gas discharge exists at low pressure, PIC-MCC method [1, 2] is a good approach for simulation of the considered physical system.

In [3] 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 [3].

In the study analysis of electrodynamics structure of the Penning gas discharge relevant for the conditions of the experiments presented in [3] 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 macro-particle [1, 2]. Macro-particle is a computational particle that simulates behaviour of a large number of real plasma particles (electrons or ions). Macro-particles follow the trajectory of real particles in the plasma since the Lorentz force depends only on the charge-to-mass ratio [4]. The movement of macro-particles 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 [5].

For the numerical solution of the Penning gas discharge problem numerical model based on 2D/3D electrostatic PIC-MCC method was used. VSim [6] software 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.

![Figure 1. PIC-MCC computational cycle (figure is taken from [7]).](image)

3. Problem formulation for simulation of experiments [3]

Validation of the numerical model is performed on the basis of experiments, conducted in University of California, Berkley [3]. In the figure 2a schematic view of experimental setup is shown.

![Figure 2. Schematic view of the Penning gas discharge.](image)

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 2 mm. Electrodes of the discharge chamber are made of aluminum. External magnetic field in the system is
created by an electromagnetic coil. This allowed varying the magnetic induction in the range of 200–500 G. In the experiments molecular hydrogen was used. The pressure of the gas was varied in the range of 0.8±1.0 mTorr. Anode potential was changed in the range 600-800 V. In the experiments dependence of the discharge current on the magnetic induction was measured (figure 3). From figure 3 it can be seen that as the magnetic field increased from 200 G to 300 G, the discharge current increased. When the magnetic field was about 300-350 G, there was some fluctuation of the discharge current. And with an increase in the magnetic field above 350 G, the discharge current decreased. It turns out that there is some optimal value of the magnetic field at which the discharge current is maximum. This work attempts to answer why there is an optimal value of the magnetic field through simulation.

Figure 3. Experimental measurement of the dependence of the discharge current on the axial magnetic field (figure is borrowed from [3]).

For numerical calculations, the Penning discharge shown in figure 2b is completely identical to the Penning discharge from [3]. For numerical calculations, the Penning discharge consisted of an anode, cathode, anti-cathode and a shell. The voltage at the anode for all calculations was 800 V. The voltage at the cathode and anticathode was 0 V (they are grounded). The diameter of the hole in the anticathode was 2 mm. The calculations were performed for molecular hydrogen under a pressure of 0.8 mTorr. The magnetic field was directed along the Oz axis and varied in the range from 200 G to 500 G.

With such parameters of the Penning discharge, the characteristic value of electron temperature $T_e \sim 10 \div 20$ eV should be expected, with an electron concentration of about $n_e \sim 2 \times 10^{16}$ m$^{-3}$. Knowing the magnetic field, the characteristic values of the electron temperature and their concentration, we can estimate [8–15]: Debye radius ($\lambda_D$), electron plasma frequency ($\omega_{pe}$), electron cyclotron frequency ($\omega_{ce}$). These values impose a limit on the size of the grids and the time step for the PIC–MCC method [16–17]. Thus, we obtain the following restrictions for PIC–MCC:

- Maximum cell size:
  \[ \Delta x_{\text{max}} < 3.4 \cdot \lambda_D [m] = 3.4 \cdot 7433 \cdot \frac{T_e [eV]}{\sqrt{n_e [m^{-3}]}} \sim 0.57 \text{ mm} \]

- Maximum time step limited by the plasma frequency of the electron:
  \[ \Delta t_{\text{max}} < \frac{0.2}{\omega_{pe}} = \frac{0.2}{5.64 \times 10^4 \sqrt{n_e [cm^{-3}]}} \sim 25 \text{ ps} \]

- Maximum time step limited by the cyclotron frequency of the electron:
  \[ \Delta t_{\text{max}} < \frac{0.2}{\omega_{ce}} = \frac{0.2}{1.76 \times 10^7 \cdot \beta [G]} \sim 23 \text{ ps} \]
For calculations, structured rectangular grids were used. Computational mesh is uniform (no thickening). For 2D calculations, the cell size was 0.25 mm and number of cell was ~ 20000. 3D calculations are very laborious and time consuming. Therefore, the cell size for 3D calculations was 0.50 mm and 0.33 mm. A mesh measuring 0.50 mm was used for faster results. For all numerical simulations time step was 10 ps.

Three kinds of macro-particles were taken into account: electrons, $H_2^+$ molecular ions and $H^+$ atomic ions. At the beginning of the numerical simulation ~100 000 electrons and ~100 000 $H_2^+$ ions were placed in the anode cylindrical region. Initial value of charged particles density is $10^{15} \text{m}^{-3}$. Initial velocities of the macro-particles were sampled using Maxwell distribution at temperature 300 K.

Elementary processes accounted for in the study were:

- elastic electron scattering on $H_2$ molecules ($e + H_2 \rightarrow e + H_2$) [18]
- ionization of $H_2$ molecules by electrons ($e + H_2 \rightarrow H_2^+ + e + e$) [18]
- $H^+$ charge exchange on $H_2$ molecules ($H^+ + H_2 \rightarrow H + H_2^+$) [19]
- $H^+$ momentum exchange on $H_2$ molecules ($H^+ + H_2 \rightarrow H^+ + H_2$) [20]
- impact ionization of $H_2$ molecules by $H^+$ ($H^+ + H_2 \rightarrow H^+ + H_2^+ + e$) [19]
- $H_2^+$ charge exchange on $H_2$ molecules ($H_2^+ + H_2 \rightarrow H_2 + H_2^+$) [19]
- $H_2^+$ momentum exchange on $H_2$ molecules ($H_2^+ + H_2 \rightarrow H_2^+ + H_2$) [20]
- impact ionization of $H_2$ molecules by $H_2^+$ ($H_2^+ + H_2 \rightarrow H_2^+ + H_2^+ + e$) [21]
- ionization of $H_2$ molecules by electrons with creating $H^+$ ($e + H_2 \rightarrow H^+ + H + e + e$) [21].

The data on the cross-section for these processes were taken from [18-23] and shown in figure 4. In the following section results of the validation of the numerical model presented above on the basis of the experiments described in [3] for various magnetic induction are going to be presented and analyzed.

![Figure 4](image-url). Cross-sections of processes used in the calculations (Here: 1 - elastic electron scattering on $H_2$ molecules; 2 - ionization of $H_2$ molecules by electrons; 3 - $H^+$ charge exchange on $H_2$ molecules; 4 - $H^+$ momentum exchange on $H_2$ molecules; 5 - impact ionization of $H_2$ molecules by $H^+$; 6 - $H_2^+$ charge exchange on $H_2$ molecules; 7 - $H_2^+$ momentum exchange on $H_2$ molecules; 8 - impact ionization of $H_2$ molecules by $H_2^+$; 9 - ionization of $H_2$ molecules by electrons with creating $H^+$).
4. Numerical results of Penning gas discharge simulation

Results of numerical simulation of Penning gas discharge at conditions relevant to experiments [3] are presented in this section. In details we will show and analyze results obtained at $B_z = 200 \div 500$ G. And the difference between 2D simulation and 3D is also discussed.

The calculations indicated that plasma tends to stationary state in 2D and 3D cases. Number of macro-electrons in stationary state was about 0.5 millions in 2D and ~ 1 million in 3D cases. Weight of each macro-particle: for 2D case and mesh 0.25 mm was 100000; for 3D case and mesh 0.50 mm was 50000; for 3D case and mesh 0.33 mm was 20000.

The distribution of fields, as well as the concentration of charged particles for 3D, will be represented as a projection of these fields on the XY and YZ plane in the sometime step. Moreover, these planes (XY and YZ) are in the middle of the Penning discharge. This is necessary to image the disturbance of axial symmetry.

In the figure 5 distributions of the electric field potential $\varphi$ [V] in the stationary state are presented for 2D case for different magnetic field. It is easy to observe that the area where the potential reaches a minimum (~ 50 V) varies depending on the magnetic field. In this region electric field has only its z-component. Potential rises to the anode which is obvious, however one can observe rise of the potential near the axis of symmetry (up to ~ 100 V).

![Figure 5. Potential distribution in 2D simulation for different magnetic field (Mesh 0.25 mm). Units for legend: [V]. Here: a – $B = 250$ G; b – $B = 300$ G; c – $B = 350$ G; d – $B = 400$ G; e – $B = 450$ G; f – $B = 500$ G.](image)

In the figure 6 distribution of the electric field potential $\varphi$ [V] in the stationary state are presented for 3D case, different magnetic field and mesh. It should be noted that in 3D case, a disturbance of the axial symmetry of the potential is observed. Moreover, with increasing magnetic field, axial symmetry breaking increases. In strong magnetic fields (400 G and above), a precession of the potential minimum around the axis of symmetry is observed. The difference between the potential distribution for meshes 0.50 mm and 0.33 mm is observed only for magnetic fields above 450 G. Most likely, that
a mesh of 0.50 mm in size poorly reproduces the electric field gradient; therefore, small deviations are observed for different meshes.

**Figure 6.** Potential distribution ($\phi$) in 3D simulation. Units for legend: [V].

Here: a, e, i, m, q, u – $\phi$ on plane XY for mesh 0.50 mm and different B; b, f, j, n, r, v – $\phi$ on plane YZ for mesh 0.50 mm and different B; c, g, k, o, s, w – $\phi$ on plane XY for mesh 0.33 mm and different B; d, h, l, p, t, x – $\phi$ on plane YZ for mesh 0.33 mm and different B.
In the Figure 7 distributions of the value electrons densities in the computational area is presented for 2D case and different magnetic field. In magnetic fields from 250 to 400 G, two peaks are observed in the distribution of the electron density. The main peak is located near the axis of symmetry. A weaker second peak is observed in the near-anode region. At the same time, as the magnetic field increases, the electron concentration at the second peak increases. For strong magnetic fields (450÷500 G), a third peak begins to form in the concentration of electron density, which lies between the previous peaks.

The distributions of the value electrons densities in the stationary state are presented on the figure 8 for 3D case, different magnetic field and mesh. With weak magnetic fields (200÷300 G), the distribution of the electron concentration is fairly uniform. There is a slight increase in the concentration of electrons near the axis of symmetry, which fluctuates in time. At high magnetic fields (350÷500 G), strong axial symmetry breaking is observed for the electron concentration distribution. At the same time, this distribution rotates around the axis of symmetry in time, preserving its structure. The results obtained for grids with sizes of 0.50 mm and 0.33 mm are consistent. Small deviations can be explained by the coarseness of the mesh and the small number of particles. But a larger number of particles will greatly complicate the calculations.
Figure 8. Electrons density distribution ($n_e$) in 3D simulation. Units for legend: electrons in m$^{-3}$.

Here: a, e, i, m, q, u – $n_e$ on plane XY for mesh 0.50 mm and different B; b, f, j, n, r, v – $n_e$ on plane YZ for mesh 0.50 mm and different B; c, g, k, o, s, w – $n_e$ on plane XY for mesh 0.33 mm and different B; d, h, l, p, t, x – $n_e$ on plane YZ for mesh 0.33 mm and different B.
Figure 9 shows the distribution of molecular ions densities ($H_2^+$) in the computational area for 2D case and different magnetic field. The distribution of $H_2^+$ in computational area reaches the maximum near the axis of symmetry and then falls to the anode. The region occupied by molecular ions increases with increasing magnetic field. But this area is limited. This is clearly seen from figure 9 with strong magnetic fields. The main part of the molecular ions ($H_2^+$) is concentrated in a cylinder with a radius of 6-8 mm at $B = 500$ G.

![Molecular ions ($H_2^+$) density distribution in 2D simulation (Mesh 0.25 mm). Units for legend: $H_2^+$ in m$^3$.](image)

Here: a – $B = 250$ G; b – $B = 300$ G; c – $B = 350$ G; d – $B = 400$ G; e – $B = 450$ G; f – $B = 500$ G.

In the figures 10 the distributions of molecular ions densities ($H_2^+$) in the computational area is presented for 3D cases and different magnetic field. The main part of molecular ions ($H_2^+$) is concentrated in a cylinder with a radius of 5-6 mm for magnetic field 300 G and above. The distribution of the ions in this cylinder is not uniform and fluctuates in time. There is good agreement between the results obtained on the grid size of 0.50 mm and 0.33 mm. In addition, for magnetic fields above 300 G, spokes are observed in the distribution of molecular ions. In time, these spokes rotate. This is clearly seen in figure 10 for calculations on a mesh of 0.50 mm and 0.33 mm. The possibility of the presence of such spokes is discussed in [24]. But for a more detailed study of the spokes, it is necessary to increase the number of macro-particles in the calculations.

In the figure 11 distributions of atomic ions densities ($H^+$) in the computational area is presented for 2D case and different magnetic field. Concentration of $H^+$ is small. That is why; there are distributions of number densities of atomic ions only for 2D case. Concentration of $H^+$ is near ~ 5 percent of $H_2^+$ ions for 2D and 3D cases. Maximum of atomic ions concentration reaches near the axis.
Figure 10. Molecular ions (H$_2^+$) density distribution in 3D simulation. Units for legend: H$_2^+$ in m$^3$.

Here: a, e, i, m, q, u – concentration H$_2^+$ on plane XY for mesh 0.50 mm and different B; b, f, j, n, r, v – concentration H$_2^+$ on plane YZ for mesh 0.50 mm and different B; c, g, k, o, s, w – concentration H$_2^+$ on plane XY for mesh 0.33 mm and different B; d, h, l, p, t, x – concentration H$_2^+$ on plane YZ for mesh 0.33 mm and different B.
Figure 11. Atomic ions \((\text{H}^+)\) density distribution in 2D simulation (Mesh 0.25 mm). Units for legend: \(\text{H}^+\) in \(\text{m}^3\). (Here: a – \(B = 250\) G; b – \(B = 300\) G; c – \(B = 350\) G; d – \(B = 400\) G; e – \(B = 450\) G; f – \(B = 500\) G).

As described earlier, the electron temperature in the Penning discharge can be estimated at about 10÷15 eV. Figure 12 shows the histogram of the electrons energy distribution with low energy (from 0 to 50 eV) for the 2D and 3D cases. The histogram of the electrons energy distribution can be described by the Maxwell distribution function which correlated with the electrons middle temperature. From figure 12 the electrons middle temperature can be estimated at about 10÷15 eV for the 2D case and about 15÷20 eV for 3D case. Small deviations in the middle temperature of electrons are possible due to the fact that for the 3D case the number of macro-particles is not large.

Figure 12. Electron \((e)\) energy distribution diagram. Here: a – 2D case with mesh 0.25 mm; b – 3D case with mesh 0.50 mm; c – 3D case with mesh 0.33 mm.
**Figure 13.** Current on different elements of Penning in 2D simulation (Mesh 0.25 mm) with magnetic field $B = 300$ G. Here: a – e current on Anode; b - e current on Cathode; c - e current on Anticathode; d – current ($H_2^+ / H^+$) on Anode; e - current ($H_2^+ / H^+$) on Cathode; f - current ($H_2^+ / H^+$) on Anticathode.

**Figure 14.** Current on different elements of Penning in 3D simulation (Mesh 0.50 mm) with magnetic field $B = 300$ G. Here: a – e current on Anode; b - e current on Cathode; c - e current on Anticathode; d – current ($H_2^+ / H^+$) on Anode; e - current ($H_2^+ / H^+$) on Cathode; f - current ($H_2^+ / H^+$) on Anticathode.
In the figure 13 electron and ions \((H_2^+/H^+)\) current on different elements of Penning is presented for 2D case and for magnetic field equal 300 G. The current fluctuation is small in the 2D case, because macro-particles in the simulation are enough. The main part of the electrons current falls on the anode. Electron current on anode in is near 4.3 mA and a good agreement with experimental results [3]. Electron current on cathode and anticathode in is not very much and consist near 40 mA. The current of molecular ions is distributed approximately equally to the cathode and anticathode. The molecular ions current on the anode is extremely low. The current of atomic ions is about 5 percent of the current of molecular ions and is distributed in the same way.

In the figures 14-15 electrons and ions \((H_2^+/H^+)\) current on different elements of Penning is presented for 3D cases and for magnetic field equal 300 G. The current fluctuation is much in the 3D cases, because macro-particles in the simulation are not many. Figures 14-15 show that the current of electrons to the cathode and anode can be from 300 to 600 mA, which differs from 2D case. Also note that the electron current to the anode is different for different meshes.

In the figure 16 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 16) that behavior of the current with increasing magnetic field is no monotonic. 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 [25] which might indicate that this is general behavior (not some feature of the considered experimental data) of current in dependence of the magnetic field.

Our calculations showed that a similar behavior of the discharge current is observed in the simulation. Such a behavior of the discharge current from the magnetic field is due to the disturbance of the axial symmetry of the field \(\phi\) and the distribution of electrons (see figure 6, 8). Moreover, the
disturbance of the axial symmetry of the field $\phi$ and the electron density is observed for a magnetic field above $300 \div 350$ G, which is in good agreement with experiment. Also, if axial symmetry is disturbance, the field $\phi$ and electron density form stable formations that rotate around the axis in time. Figure 16 shows the difference for discharge current in 3D modeling for different mesh sizes. This may be due to the fact that the coarse mesh does not reproduce the field gradients well.

Using of the 2D PIC-MCC method does not allow simulating this effect, because in this method there is no possibility to model the disturbance of axial symmetry. Therefore, the discharge current only increases with increasing magnetic field for the 2D case.

Mass spectrum of the extracted current from the Penning ion source was measured in the experiments [3]. This measurement has shown the presence of hydrogen atoms in the extracted current. Our calculations showed that using processes from [18-21] can be get current of atomic ions near 5 percent of molecular ions current.

Figure 16. Comparison of experimental and numerical data.

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. Electrodynamics structure of the Penning gas discharge at pressure $p = 0.8$ mTorr, voltage on anode = $800$ V and $B = 200 - 500$ G were obtained and analyzed. Distribution of potential, electric field, charged particles densities, temperatures and energy distribution functions are presented. All simulations were calculated in 2D and 3D cases. It was compared results for 2D and 3D simulations.

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 (see figure 16).

The experiment [3] show that there exists $I_{\text{max}}$ and corresponding $B_{\text{max}}$ after which further increase in B leads to decrease in I. Our calculations showed that a similar behavior of the discharge current is observed in the simulation. Such a behavior of the discharge current from the magnetic field is due to the disturbance of the axial symmetry of the field $\phi$ and the distribution of electrons (see figure 6, 8).
Moreover, the disturbance of the axial symmetry of the field $\phi$ and the electron density is observed for a magnetic field above $300-350$ G, which is in good agreement with experiment [3] (see figure 16). Also, if axial symmetry is disturbance, the field $\phi$ and electron density form stable formations that rotate around the axis in time. The difference for discharge current in 3D modeling for different mesh sizes is observed. This may be due to the fact that the course mesh does not reproduce the field gradients well.

Spokes are observed in the distribution of molecular ions for 3D modeling. In time, these spokes rotate. This is clearly seen in figure 10 for calculations on a mesh of 0.50 mm and 0.33 mm. The possibility of the presence of such spokes is discussed in [24]. But for a more detailed study of the spokes, it is necessary to increase the number of macro-particles in the calculations.

Using of the 2D PIC-MCC method does not allow simulating this effect, because in this method there is no possibility to model the disturbance of axial symmetry. Therefore, the discharge current only increases with increasing magnetic field for the 2D case. Also our calculations showed that using processes from [18-21] can be get current of atomic ions near 5 percent of molecular ions current.

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