Calculation of the Fraction of Atomic Hydrogen in the Penning Discharge Plasma using the PIC–MCC Method

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Abstract. In this paper, the process of dissociative ionization is incorporated into the existing model of Penning discharge in molecular hydrogen. The analysis of studies for the selection of effective cross-sections for this process is performed. The results of calculations with the following parameters are given: working gas - H2, p = 0.8 mTorr, V = 600 V, B = 200-500 G. Comparison of calculated relative shares of atomic and molecular ions with experimental data obtained at the University of California, Berkeley has been performed.

1. Introduction
Penning discharge [1] can be characterized as a glow discharge, which exists only in the presence of an external magnetic field in the discharge chamber. This type of discharge has found application in a wide range of areas, such as medicine, aerospace industry and many others [2]. In this type of discharge plasma is generated at the center of the discharge chamber by the electrons. A small amount of studies is devoted to the development of full-fledged numerical model for simulation of the electrodynamic structure of the Penning gas discharge plasma.

The particle-in-cell method with Monte-Carlo collision method is one of the possible numerical approaches that can be used for simulating plasma processes in the Penning gas discharge. Previously computer code [3] was developed that implements 2D/3V PIC-MCC method, which was tested by comparison with numerical and experimental data [3, 4]. But in the [4], only the processes of ionization of the hydrogen molecules by electrons and elastic scattering of electrons on the hydrogen molecules were considered. It was revealed in [2] that during the burning of the Penning discharge in a gas consisting of molecular hydrogen, 3 types of positive charged particles were formed: two types of molecular hydrogen ions and atomic hydrogen ions. It is worth noting that the ratio of H2+ to the total amount of all types of ions was about 90%, and the number of triatomic hydrogen ions was less than 1%.

In the papers [5, 6] the author has formed full and simplified kinetic scheme for describing the kinetics of ionization of hydrogen in Penning gas discharge plasma. In the papers, the author emphasizes that the main process of generation of atomic hydrogen ions is the dissociative ionization. Thus for more efficient validation we need to add the processes of dissociative ionization to the existing scheme:
2. Numerical model of dissociative ionization

In the papers [5, 6] the author has defined a full and simplified kinetic scheme for determining the processes that occur during the burning of the Penning discharge. In this work, we consider only the processes by which atomic ions are produced. A list of these processes is presented below:

1. \[
H_2(X^1\Sigma_g^+, v_i) + e \rightarrow H_2^+(X^2\Sigma_g^+) + 2e \rightarrow H(1s) + H^+ + 2e
\]

2. \[
H_2(X^1\Sigma_g^+, v_i) + e \rightarrow H_2^+(\tilde{1}^2\Sigma_g^+) + 2e \rightarrow H(1s) + H^+ + 2e
\]

3. \[H + e \rightarrow H^+ + e + e\]

4. \[H_2^+ + H \rightarrow H_2 + H^+\]

In the paper [6], the author highlighted that the processes of dissociative ionization 1 and 2 as main source of atomic hydrogen ions. The processes 1 and 2 are two-step. However it is known that the intermediate step finishes extremely quickly. Then the processes of dissociative ionization may be considered as single step process. It is also possible to simplify the scheme, without dividing the process of dissociative ionization into 2 types. Ultimately, both of these processes can be described as:

\[
H_2(X^1\Sigma_g^+, v_i) + e \rightarrow H + H^+ + 2e
\]

In this work the numerical model of dissociative ionization is based on methodology of development of collision models of elementary processes for the Monte-Carlo method described in [7] and [8].

Scheme of modeling of the process of dissociative ionization is similar to the scheme of modeling of ionization or dissociation. Dissociative ionization is treated like inelastic collision and the energy balance equation can be described as:

\[
\epsilon_i + \epsilon_{ej} + \epsilon_i = \epsilon_{inc} + \epsilon_N - \epsilon_{ion}
\]

Where \( \epsilon_i \) is the energy of the incident electron, \( \epsilon_{ej} \) is the energy of the ejected electron, \( \epsilon_N \) is the energy of the target neutral atom and \( \epsilon_i \) is the energy of the created ion.
In these reactions, the incident electrons lose at least the threshold energy and scatter through angles $\chi$ and $\phi$ determined as:

$$\phi = 2\pi R$$  \hspace{1cm} (2)$$

$$\chi = \text{arccos} \left( \frac{2 + \varepsilon_{\text{inc}} - 2(1 + \varepsilon_{\text{inc}})^2}{\varepsilon_{\text{inc}}} \right)$$  \hspace{1cm} (3)$$

Where $\chi$ - polar scattering angle, $\phi$ - azimuthal scattering angle and $R$ and $S \in [0, 1]$ are random numbers. As soon as we calculate the polar and azimuthal scattering angles, we can determine the vector of direction of the scattered velocity by geometric considerations. We can also calculate the energy loss of the electron in a scattering event as:

$$\Delta \varepsilon = \frac{2m}{M} (1 - \cos \chi)$$  \hspace{1cm} (4)$$

where $m$ and $M$ are the electron mass and the mass of a neutral particle, respectively. Due to the large mass ratio of the ions to the electron, it can be assumed that the momentum of the incident electron is much smaller than the momentum of the neutral atoms. Thus one can assume that:

$$\varepsilon_i = \varepsilon_{N}$$

and

$$\varepsilon_{\text{st}} + \varepsilon_{e} = \varepsilon_{\text{inc}} - \varepsilon_{\text{ion}}$$

After this we can find the energy of the ejected electron by solving following equation:

$$R = \frac{\int_{0}^{\varepsilon_i} \sigma(\varepsilon_{\text{inc}}, \varepsilon_{e}, \varepsilon_{\text{ion}}) d\varepsilon_{e}}{\int_{0}^{\varepsilon_{\text{st}} - \varepsilon_{\text{ion}}} \sigma(\varepsilon_{\text{inc}}, \varepsilon_{e}, \varepsilon_{\text{ion}}) d\varepsilon_{e}}$$  \hspace{1cm} (5)$$

Cross sections for dissociative ionization in hydrogen was taken from [9–16] papers. Comparative chart for cross sections is presented in figure 2. Calculations in our study will be performed using cross-sections presented in [11]. Energy threshold for the dissociative ionization process was given in [17] and equals to 18.1 eV.

![Cross sections for dissociative ionization in molecular hydrogen.](image)

**Figure 2.** Cross sections for dissociative ionization in molecular hydrogen.

3. **Numerical results**

For calculation of the spatial distribution of molecular and atomic hydrogen ions in the discharge chamber the following Penning gas discharge parameters were studied: working gas - H$_2$, ...
$p = 0.8 \ \text{mTorr}, \ V = 600 \ \text{V}, \ B = 200-500 \ \text{G}$. Considered gas discharge parameters correspond to the data obtained in experiments performed at the University of Berkeley, California. Results presented in the work are obtained using the assumption that magnetic field inside the discharge chamber is uniform. Study of the electrodynamic structure of the Penning gas discharge in non-uniform magnetic field was performed in [18].

In the study numerical simulation of two-dimensional electrodynamic structure of Penning discharge plasma is performed using 2D/3V axisymmetric electrostatic particle-in-cell Monte-Carlo collision (PIC–MCC) computer code. The algorithmic structure of the single time step in the framework of the method is presented in figure 3. PIC–MCC method includes the concept of macroparticles, which model large number of charged particles. Whole process is self-consistent because the movement of macroparticles changes the distribution of electromagnetic field in the system and electromagnetic field determines the force acting on the particles.

![Figure 3. PIC-MCC computational cycle.](image)

Geometry of computational domain corresponds to the geometry of the discharge chamber used in the experiments [2]. Uniform unstructured triangular mesh (see figure 4) was created in the computational domain. It consists of 2648 nodes and 5099 triangles. Numerical simulation was performed at the anode voltage 600 V (cathodes are grounded).

![Figure 4. Geometry of the discharge chamber and computational mesh.](image)

Three types of macroparticles were taken into account: electrons, diatomic molecular ions and atomic ions of hydrogen. At the beginning of numerical simulation 120000 electrons, 60000 diatomic
ions of hydrogen and 60,000 atomic ions of hydrogen were placed in the cylindrical region in the center of simulation area. Initial number density of negative charged particles was $5 \cdot 10^8$ cm$^{-3}$. Initial number density of each positive charged particles species was $2.5 \cdot 10^9$ cm$^{-3}$. Initial velocities of the macroparticles were sampled by Maxwellian distribution at temperature 300 K. Time step for calculation has taken as $4 \cdot 10^{-12}$ seconds.

Elementary processes accounted in the study are: elastic electron scattering on H$_2$ molecules, ionization of H$_2$ molecule by electron impact, and the dissociative ionization of H$_2$ molecule by electron impact. Also the mechanism of ion-electron emission from the cathode was taken into account.

Spatial distributions of number density of molecular ions of hydrogen are presented in figures 5–8.

**Figure 5.** Spatial distribution of diatomic molecular ions of hydrogen density $n_{\text{H}_2^+}$ [cm$^{-3}$] in steady state, $B_z = 0.023$ T.

**Figure 6.** Spatial distribution of diatomic molecular ions of hydrogen density $n_{\text{H}_2^+}$ [cm$^{-3}$] in steady state, $B_z = 0.030$ T.

**Figure 7.** Spatial distribution of diatomic molecular ions of hydrogen density $n_{\text{H}_2^+}$ [cm$^{-3}$] in steady state, $B_z = 0.041$ T.

**Figure 8.** Spatial distribution of diatomic molecular ions of hydrogen density $n_{\text{H}_2^+}$ [cm$^{-3}$] in steady state, $B_z = 0.045$ T.
In the figures 5–8 one can observe that increase of the magnetic field induction leads to the shift of the region of maximum number density of $\text{H}_2^+$ from the axis of symmetry to the anode. The value of the maximum number density of $\text{H}_2^+$ also increases with increasing induction of the magnetic field.

Spatial distributions of number density of atomic hydrogen ions are presented in figures 9–12. One can observe that as in the case of $\text{H}_2^+$ ions increase of the magnetic field induction leads to the shift of the region of maximum number density of $\text{H}^+$ ions from the axis of symmetry to the anode. The effect of the shifting of the region of maximum number density with varying magnetic field is more prominent in the case of $\text{H}^+$ ions than in the case of $\text{H}_2^+$ ions. Generally it may be noted that spatial distribution of $\text{H}_2^+$ ions number density is more uniform along the axial coordinate than the spatial distribution of $\text{H}^+$ ions number density.

**Figure 9.** Spatial distribution of atomic ions of hydrogen density $n_{\text{H}^+} \text{[cm}^{-3}\text{]}$ in steady state, $B_z=0.023\ \text{T}$.

**Figure 10.** Spatial distribution of atomic ions of hydrogen density $n_{\text{H}^+} \text{[cm}^{-3}\text{]}$ in steady state, $B_z=0.030\ \text{T}$.

**Figure 11.** Spatial distribution of atomic ions of hydrogen density $n_{\text{H}^+} \text{[cm}^{-3}\text{]}$ in steady state, $B_z=0.041\ \text{T}$.

**Figure 12.** Spatial distribution of atomic ions $n_{\text{H}^+} \text{[cm}^{-3}\text{]}$ of hydrogen density in steady state, $B_z=0.045\ \text{T}$.
In the figures 13–16 spatial distributions of the temperature of $H_2^+$ ions in [eV] are presented. As well as in the case of the number density one can observe dependence of the position of the region of maximum temperature on the magnetic field. The value of the maximum temperature increases with increasing magnetic field induction and reaches 170 eV. One can notice that spatial distribution of temperature of the molecular hydrogen ions is uniform along the axis of symmetry. The variations are observed in the radial direction.

Figure 13. Spatial distribution of temperature [eV] of diatomic ions of hydrogen in steady state, $B_z=0.023$ T.

Figure 14. Spatial distribution of temperature [eV] of diatomic ions of hydrogen in steady state, $B_z=0.030$ T.

Figure 15. Spatial distribution of temperature [eV] of diatomic ions of hydrogen steady state, $B_z=0.041$ T.

Figure 16. Spatial distribution of temperature [eV] of diatomic ions of hydrogen in steady state, $B_z=0.045$ T.

In the figures 17–20 spatial distributions of the temperature of $H^+$ ions in [eV] are presented. Numerical calculations predict that maximum temperature of the atomic hydrogen ions is about 210 eV, which is higher than the maximum temperature of $H_2^+$ ions. The effect of dependence of the position of the region of maximum temperature on the magnetic field is observed in these distributions.
as well. As in the case of $\text{H}_2^+$ ions, temperature of $\text{H}^+$ ions mainly varies along radial coordinate and quite uniform along the axis of symmetry.

**Figure 17.** Spatial distribution of temperature [eV] of atomic ions of hydrogen in steady state, $B_z = 0.023$ T.

**Figure 18.** Spatial distribution of temperature [eV] of atomic ions of hydrogen in steady state, $B_z = 0.030$ T.

**Figure 19.** Spatial distribution of temperature [eV] of atomic ions of hydrogen in steady state, $B_z = 0.041$ T.

**Figure 20.** Spatial distribution of temperature [eV] of atomic ions of hydrogen in steady state, $B_z = 0.045$ T.

In the figure 21 number of macroparticles that represent atomic and molecular hydrogen ions at four different magnetic fields are shown. Using presented figures one can estimate the fraction of $\text{H}^+$ ions in the Penning gas discharge plasma at considered conditions. According to the numerical results fraction of $\text{H}^+$ ions is almost independent of the magnetic field induction and equals to $5\div6$ %. Experimental results obtained in University of California, Berkley indicate that measured proton fraction typically falls within the range of $5\div10\%$, showing some variation with the variation in the axial magnetic field [2]. Thus there is a qualitative agreement between experimental and numerical results.

![Amount of ions in steady state](image)

**Figure 21.** Number of macroparticles that represent hydrogen molecular and atomic ions at different magnetic field $B_z=0.023\div0.045$ T (from left to right).

In the figure 22 energy distribution functions (EDF) of charged particles are presented. The EDF can be calculated according to the following formula:

$$ f(\nu) = \frac{dN}{N d\nu} $$
One can see from the figure 22 that the behavior of the EDF of H\(^+\) ions is similar to EDF of molecular hydrogen ions.

![Figure 22. Energy distribution function of electrons and ions in steady state](image)

4. Conclusion
In the study numerical model for the simulation of Penning gas discharge in molecular hydrogen is extended by incorporation of the process of dissociative ionization of H\(_2\) molecule. The model is applied for the analysis of experiments conducted in the University of California, Berkley. Electrodynamic structure of the Penning gas discharge at pressure \(p = 0.8\) mTorr, \(V = 800\) V and \(B_z = 0.023\)÷0.045 T was obtained and analyzed. Distributions of charged particles number densities, temperatures and energy distribution functions are presented. Fraction of atomic hydrogen ions in the Penning gas discharge plasma is obtained using proposed numerical model and compared against known experimental data. The agreement between experimental and numerical results is satisfactory.

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