Plasma Optimization in a Multicusp Ion Source by Using a Monte Carlo Simulation

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(Received 26 December 2012, in final form 22 April 2013)

A Monte Carlo simulation code has been developed to optimize the number of magnets confining the plasma in the H- multicusp ion source. This code improves the existing drawbacks in the particle studio CST program and predicts the lifetime of primary electrons and the effects of collisions of electrons and hydrogen gas atoms. In this simulation are found 12 cusps to provide the highest plasma intensity in our configuration. Finally, our developed code is validated by simulating the experimentally-tested KSTAR ion-source configuration and semi-empirical equation.

PACS numbers: 21.60.Ka, 29.25.Ni, 52.20.Fs
Keywords: Multicusp ion source, Magnetic confinement, Electron trajectory
DOI: 10.3938/jkps.63.0

I. INTRODUCTION

Multicusp ion sources have been widely used in particle accelerators [1-3] and fusion reactors [4]. Permanent magnets can be utilized to improve the density and the uniformity of DC discharge plasma. The underlying idea of a set of permanent magnets is to force the electrons to spend a large portion of their flight path inside the plasma. In this way, the probability of a collision with a neutral gas molecule in the plasma is enhanced. This procedure increases the probability of an ionizing process, i.e., the current of a negative ion beam. Experimental results indicate that the large increase in density in this type of source is mainly due to the confinement of the primary ionizing electrons by the magnetic fields of the magnets. The confinement of ions, however, is found to be significantly weaker. Plasma can be lost to the line cusps and to the regions between the cusps [5].

In this work, we analyze the CYCLONE30 multicusp negative ion source [6] by using a 3D Monte Carlo simulation code to trace electron trajectories. A realistic geometry and multicusp magnetic field configuration are taken into account, and the electron trajectories are followed. The neutral gas atom is hydrogen in the present study. In this article, we focus our attention mainly on processes the H- volume is produced. The types of collisions that we calculated are vibrational excitation of hydrogen by fast electrons, dissociative attachment to highly vibrationally-excited molecules and ionization related to production of the H- ion. Our simulation illustrates the existence of an optimum point in choosing the number of permanent magnets for confining the plasma.

II. SIMULATION CODE

The electron trajectories are calculated numerically by solving the 3D equation of motion

\[ m \frac{dV}{dt} = q(E + V \times B) , \]

where \( m \), \( V \), \( q \), \( E \), and \( B \) are the electron’s mass, velocity, charge, and the electric and magnetic fields, respectively. The electric field is neglected in the above equation because it is negligibly small over the entire plasma region. When \( x \) is the position vector, the definition of the velocity vector is given by

\[ dx/dt = V . \]

We have used a Runge-Kutta integrator to solve the two equations of motion above.

Here we only consider production processes to follow electron orbits in the chamber. The following production processes and ionization are taken into account by the Monte Carlo method in each time step [7]:

**Vibrational excitation of H\(_2\)**

\[ \text{H}_2 + e_{\text{fast}} \rightarrow \text{H}_2^* (v'' \geq 5) + e , \]

**Dissociative attachment**

\[ \text{H}_2^* (v'') + e_{\text{slow}} \rightarrow \text{H}^- + \text{H} . \]

The vibrational levels (\( v'' \)) are also taken into account because the reaction cross-sections are also \( v'' \) dependent [8]. Dissociative electron attachment to
vibrationally-cold \( \text{H}_2 (\nu'' = 0) \) molecules is known to have a very small cross section \( 10^{-21} \text{ cm}^2 \).

The experiment of Allan and Wong [9] and the theoretical calculations of Wadehra and Bardsley [10] showed that the DA (dissociative attachment) cross section increases by five orders of magnitude when the hydrogen molecules are vibrationally excited from \( \nu'' = 0 \) to \( \nu'' = 5 \), and stay constant at higher \( \nu'' \). The collisions between electrons and neutral atoms are calculated by the Monte Carlo method. The collision length is the distance between two successive collisions caused by a test particle and is defined as:

\[
l = -\lambda \ln(r) ,
\]

where \( \lambda \) is the mean free path of the collision and \( r \) is a random number between 0 and 1. Because the cross sections are energy dependent, we consider three corresponding to different energies. At the beginning or after a collision, the particle starts with a speed derived from Maxwell’s speed distribution, and a random direction is chosen to continue the trajectory calculation. The following scheme is used to generate the Maxwell speed distribution of the particles for the Monte-Carlo calculation:

\[
v = \text{abs}[v_m \times \sqrt{\ln(\frac{1}{r}) + (\frac{v_m}{3})}],
\]

where \( r \) is a random number and \( v_m = \sqrt{\frac{2k_B T}{m}} \) is the most probable speed of the particle having temperature \( T \) and mass \( m \).

The mean free path \( \lambda \) for individual reaction is calculated from the reaction cross-section. Because the reaction rates and the cross sections are energy dependent, Maxwell’s speed distribution of the electrons is considered. The flight length \( \zeta \) is obtained by integrating the flight path in each time step as follows:

\[
\zeta = \int_{t_0}^{t} |V| dt .
\]

If \( \zeta \) becomes equal to \( l \), the collision process is included in that time step. Here, we assume that the hydrogen atoms fill the chamber as a neutral gas and have no kinetic energy because their thermal energy is considerably less than that of electrons.

### III. PHYSICAL MODEL OF THE MULTICUSP ION SOURCE

Figure 1 shows the simulated ion source configuration. This ion source consists of four major parts: the source body (walls of the plasma chamber), the lid which holds the filament, the magnetic filter and the puller assembly. The body of the original design of the source is a 150-mm-long, 100-mm-diameter copper cylinder around which ten columns of permanent magnets with magnetic field of 6.2 kG are mounted.

### IV. MAGNETIC FIELD CALCULATION

The complete topology of the magnetic field configuration of the ion source is calculated in a separate computer code, CST PARTICLE STUDIO [11]. Figure 2 shows a simulated magnetic field configuration.

The filament power supply has a current of 100 A and a voltage of 10 V. According to Bio-savart’s law, the magnetic field of a wire with a current of 100 A in the 2 cm surrounding the wire is calculated as follows:

\[
B = \mu_0 I / 2\pi r = \left(4\pi \times 10^{-7} \times 100\right) / \left(2\pi \times 0.02\right) = 10^{-2} T = 10 \text{ G} .
\]

As is clear from Fig. 2, near the surfaces of the magnets the magnetic field is roughly 1800 G, and in the center of
Table 1. Calculation of the total electron trajectory and number of collisions for the CYCLONE30 multicusp in different numbers of magnets.

<table>
<thead>
<tr>
<th>Sum of electron trajectory (m)</th>
<th>4</th>
<th>6</th>
<th>8</th>
<th>10</th>
<th>12</th>
<th>14</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total number of collisions</td>
<td>3309</td>
<td>3068</td>
<td>3685</td>
<td>6864</td>
<td>7070</td>
<td>3990</td>
</tr>
<tr>
<td>Average confinement time of electrons in the chamber (s)</td>
<td>2.1E-06</td>
<td>7.3E-06</td>
<td>4.9E-06</td>
<td>6.9E-06</td>
<td>7.4E-06</td>
<td>3.6E-06</td>
</tr>
</tbody>
</table>

Fig. 3. (Color online) Percentage of electrons that lost their energy completely due to interactions at a hydrogen pressure of 4 mTorr.

Fig. 4. (Color online) time of electrons.

V. SIMULATION METHOD

To the best of our knowledge, no specific simulation method has been reported yet to explore the optimal number of cusps of the magnetic field; furthermore, are lacking proper theoretical methods to economize the time and the cost of the design and the fabrication. To evaluate the performance of different cusp spacing, we simulated the total distance that electrons travel.

CST is able to track particles in an electric and magnetic field but it does not simulate the interactions of particles. Also, it provides data concerning neither the particle trajectory, position and velocity at the desired time nor the total path traveled by a particle. In order to optimize the CYCLONE30 ion source, we developed a computer program. Our developed Monte Carlo code was used to find the total distance that electrons traveled.

The process of optimization is as follow: the number of permanent magnets used to create magnetic field lines is the optimization parameter, and the chamber’s radius, height and filament position are constant. The number of magnets is varied from 4 to 14 with the geometrical specifications shown in Fig. 1. The magnetic field is calculated by using CST software and exported to our Monte Carlo code. Because of having a magnetic flux density at every point of the chamber, 5000 electrons are emitted from the filament and are allowed to leave the filament cathode in different positions, and because they have random velocity direction, they move in the magnetic field created by the surrounding magnets. The initial energy of the emitted electrons is assumed to be 200 eV in the present simulations because the discharge voltage is 200 V. Electrons collide with neutral atoms elastically or inelastically and their movement is affected by the magnetic field. In the case of inelastic collisions, electrons ionize or excite the atoms. When the electron’s energy decreases to very low energies like 1 eV, according to dissociative attachment reaction it is attached to excited hydrogen molecules or it collides with the chamber wall and leaves the chamber. In this simulation, the total length that electrons have traveled, the total number of collisions and the percentage of electrons involved in gas ionization are calculated.
Table 2. Electron trajectory and confinement time for two magnets arrangement.

<table>
<thead>
<tr>
<th></th>
<th>Axial configuration</th>
<th>Azimuthal configuration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sum of electron trajectory (m)</td>
<td>9232.27</td>
<td>42112.00</td>
</tr>
<tr>
<td>Average confinement time of electrons in the chamber (s)</td>
<td>2.6E-07</td>
<td>3.2E-06</td>
</tr>
</tbody>
</table>

Table 3. Reactions included in the model.

<table>
<thead>
<tr>
<th>Label</th>
<th>Reactions</th>
<th>(&lt; \sigma \nu &gt; (m^3 s^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>E-V</td>
<td>H(<em>2) + e(</em>{\text{fast}}) → H(_2^*) ((v'' \geq 5)) + e</td>
<td>5 × 10(^{-17})</td>
</tr>
<tr>
<td>Dissociative Attachment</td>
<td>H(<em>2^*) ((v'')) + e(</em>{\text{slow}}) → H(^-) + H</td>
<td>6.5 × 10(^{-15})</td>
</tr>
<tr>
<td>Ionization</td>
<td>H(_2^*) ((v'')) + e → H(_2^+) + 2e</td>
<td>9 × 10(^{-16})</td>
</tr>
</tbody>
</table>

VI. RESULTS AND DISCUSSION

Table 1 shows the value of the total electron path and the number of collisions of electrons with neutral gas for different numbers of magnets. As can be seen, these values are the highest for 12 magnets, which shows a super performance in comparison to the other configurations for this specific dimension. When 12 columns are employed, electron trajectories and numbers of collisions are higher. This result shows that 12 is an optimum case because electrons take more trajectory which results in more collisions, ionization, and finally more plasma density, which is the goal of this research. Electrons are stopped either due to complete loss of their energy in the process of interactions or due to collision with the chamber of ion source.

Figure 3 shows the percentage of electrons that lose their energy due to interactions in the chamber at a hydrogen pressure of 4 mTorr. The number of samples is 5000. As Fig. 3 shows the maximum percentage of electrons involved in ionization, excitation and dissociative attachment interactions occurs when the number of permanent magnets is 12.

Figure 4 shows the flight time of electrons. The total number of electrons for each simulation is 5000, and almost 90 percent of them hit the wall and stop in our simulation, but a small fraction of them collide with hydrogen molecules. As is evident in Fig. 4 when the num-

Fig. 5. (Color online) Three dimensional magnet arrangement of the ion source. (a) axial line cusp and (b) azimuthal line cusp.

Fig. 6. (Color online) Flow chart for the electron calculation.
number of magnets is 12, more electrons fly in the chamber, which entails more negative-ion current production.

**VII. CODE VALIDATION**

To validate the developed code, we adopted two methods. The first one was simulating the KSTAR ion source arrangement [12] for comparison of the experimental work with our simulation. The magnetic field of two types of magnet arrangements, axially and azimuthally, was solved by using the CST program; then, its magnetic fields were imported to our code to compare the results. We tracked the electrons in two different configurations and calculated the sum of the electron trajectories and the confinement times of electrons in both arrangements (Table 2). We concluded that the plasma intensity was higher in azimuthal magnet arrangement which was consistent with the experimental observation. The plasma chamber had a cross section of 26 × 64 cm, it was 32 cm deep, and it was surrounded by 40 Sm-Co permanent magnets with dimensions of 13 × 19 × 25 mm³ to create a cusp field around the inner wall of the chamber (Fig. 5). After solving the magnetic field, we tracked 5000 electron trajectories in our code to find the values of the confinement time and the total electron trajectory. We found that the confinement time and the electron trajectory in the azimuthal configuration were higher which led to a higher, plasma intensity.

The second validation method compared the results with the following semi-empirical equation for each reaction separately:

\[ n_e n_{H_2} < \sigma \nu >, \]

(9)

where \( n_e \) is the primary electron density, \( n_{H_2} \) is the neutral gas density and \( < \sigma \nu > \) is the reaction rate coefficient for inelastic collisions including ionization and excitation. The reaction rate coefficients for the three reactions considered in the simulation are listed in Table 3 [13]. In the real ion source \( n_e \) is \( 10^{21} \) m⁻³, which is electrons emitted by the filament and is calculated through Richardson-Dushman equation, but here we considered only 5000 particles. Also, for \( p = 4 \) mTorr, \( n_{H_2} \) is equal to 13.3 × 10¹⁹ m⁻³. The results of our calculations are equal to 4.3 × 10²⁵. The results of our calculations are also compared in Tables 4, 5 and 6. We optimistically ascertain that our results are the same order as the tabulated reaction rates by using the formula, which demonstrates that our approach is a valid procedure.

**VIII. CONCLUSION**

We developed an electron orbit simulation code, which included the phenomena of collisions between electrons and neutral atoms to optimize the cusp spacing for our ion source. In this simulation, different numbers of magnets were studied. The simulation showed a considerable improvement in the performance when 12 magnets were used. The developed approach allowed a proper theoretical method to gain an efficient configuration in multicusp which could lower the cost and decrease the design and fabrication time.

### Table 4. Reaction rates for vibrational excitation of H₂ reaction (number of collisions/m³s).

<table>
<thead>
<tr>
<th></th>
<th>4</th>
<th>6</th>
<th>8</th>
<th>10</th>
<th>12</th>
<th>14</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reaction rate from simulation</td>
<td>1.6 × 10²⁵</td>
<td>4.3 × 10²⁵</td>
<td>4.4 × 10²⁵</td>
<td>3.2 × 10²⁵</td>
<td>3.4 × 10²⁵</td>
<td>4.3 × 10²⁵</td>
</tr>
<tr>
<td>Reaction rate from equation</td>
<td>3.1 × 10²⁵</td>
<td>3.1 × 10²⁵</td>
<td>3.1 × 10²⁵</td>
<td>3.1 × 10²⁵</td>
<td>3.1 × 10²⁵</td>
<td>3.1 × 10²⁵</td>
</tr>
</tbody>
</table>

### Table 5. Reaction rates for dissociative attachment reaction (number of collisions/m³s).

<table>
<thead>
<tr>
<th></th>
<th>4</th>
<th>6</th>
<th>8</th>
<th>10</th>
<th>12</th>
<th>14</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reaction rate from simulation</td>
<td>1.6 × 10²⁷</td>
<td>1.4 × 10²⁷</td>
<td>2.2 × 10²⁷</td>
<td>1.5 × 10²⁷</td>
<td>1.5 × 10²⁷</td>
<td>1.47 × 10²⁷</td>
</tr>
<tr>
<td>Reaction rate from equation</td>
<td>3.9 × 10²⁷</td>
<td>3.9 × 10²⁷</td>
<td>3.9 × 10²⁷</td>
<td>3.9 × 10²⁷</td>
<td>3.9 × 10²⁷</td>
<td>3.9 × 10²⁷</td>
</tr>
</tbody>
</table>

### Table 6. Reaction rates for ionization reaction (number of collisions/m³s).

<table>
<thead>
<tr>
<th></th>
<th>4</th>
<th>6</th>
<th>8</th>
<th>10</th>
<th>12</th>
<th>14</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reaction rate from simulation</td>
<td>3.2 × 10²⁷</td>
<td>1.15 × 10²⁷</td>
<td>9.1 × 10²⁶</td>
<td>1.5 × 10²⁷</td>
<td>1.6 × 10²⁷</td>
<td>1.1 × 10²⁷</td>
</tr>
<tr>
<td>Reaction rate from equation</td>
<td>0.6 × 10²⁷</td>
<td>0.6 × 10²⁷</td>
<td>0.6 × 10²⁷</td>
<td>0.6 × 10²⁷</td>
<td>0.6 × 10²⁷</td>
<td>0.6 × 10²⁷</td>
</tr>
</tbody>
</table>
APPENDIX A: FLOW CHART OF CALCULATION OF AN ELECTRON

Figure 6 shows a flow chart of the calculations in the present simulations. In the first step, the emission position, the velocity vector of an electron and the free path are determined by using the Monte Carlo method. In each time step, the code first solves the equation of motion. Next, it checks whether or not a collision occurs by comparing free path $l$ and flight length $\zeta$. In the case of a collision, the scattering angle and the energy loss are calculated by using the Monte Carlo method. If the rest energy of electrons is less than the threshold values, the calculation is terminated.

REFERENCES