

Three-Dimensional Particle-in-Cell Simulation of a Miniature Microwave Discharge Ion Thruster $\mu 1$

IEPC-2013-186

*Presented at the 33rd International Electric Propulsion Conference,
The George Washington University • Washington, D.C. • USA
October 6 – 10, 2013*

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Abstract: We have developed a three-dimensional particle model for a miniature microwave discharge ion thruster $\mu 1$ to elucidate the mechanism of ECR discharges confined in a small space. The model consists of a particle-in-cell simulation with a Monte Carlo collision algorithm for the kinetics of charged particles, a finite-difference time-domain method for the electromagnetic fields of 4.2-GHz microwaves, and a finite element analysis for the magnetostatic fields of permanent magnets. Simulation results have shown that the electrons are well confined owing to the mirror magnetic fields and can be effectively heated in the ECR layer downstream of the ring antenna. The distribution of the plasma density obtained in the calculation is quite similar to that of the plasma discharge of $\mu 1$ in operation. Moreover, the numerical result of the Xe metastable distribution is also in a reasonable agreement with the experimental result.

Nomenclature

B	= magnetic field
E	= electric field
f	= microwave frequency
j	= current density
m	= mass
n	= number density
P	= power
q	= charge

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T	=	temperature
t	=	time
$\mathbf{v}$	=	velocity
ϵ_0	=	vacuum permittivity
μ_0	=	vacuum permeability
ρ	=	charge density
ϕ	=	electrostatic potential

I. Introduction

IN recent years, the worldwide interest in microspacecraft has grown to such an extent that even universities are currently able to launch and operate microspacecraft because of their low costs and short development periods. However, most microspacecraft do not have any propulsion systems, which is why they rely on passive controls, such as gravity gradient stabilization and geomagnetic attitude stabilization. If a microspacecraft had microthrusters mounted on it, we could control the microspacecraft more effectively to create a specific flight path. Owing to the limited power generation and propellant storage, high specific impulses, high-thrust efficiencies and low-power consumptions are required for microthrusters, in addition to small size and light weight.¹

Figure 1 shows a miniature ion thruster developed by the Institute of Space and Astronautical Science in Japan Aerospace Exploration Agency (ISAS/JAXA) with the purpose of solving the issues mentioned above; the ion thruster is referred to as $\mu 1$ (“mu-one”), as one of the “mu-series” microwave discharge ion thrusters developed by ISAS/JAXA, where electron cyclotron resonance (ECR) is employed for plasma discharges. Its ion source has the 250 W/A ion production cost and 37% mass utilization efficiency for 1.0 W microwave input power and 14.6 $\mu\text{g/s}$ xenon mass flow, where the neutralizer employs the identical discharge chamber and operates with a gas flow of half ion beam source. By using an ion beam source and a neutralizer, a miniature ion propulsion system (MIPS) was developed by the University of Tokyo in collaboration with the Next Generation Space Technology Research Association (NESTRA) in Japan. The EM specifications of the MIPS is evaluated at the weight of 8.1 kg (dry: 7.1 kg), volume of 39×26×15 cm³, power consumption of 39 W and thrust of 300 μN with specific impulse of 1200 s.² The MIPS is intended for the installation on a 50 kg-class spacecraft, HODOYOSHI-4, which is scheduled to be launched in early 2014.

On the other hand, there are still some physical phenomena to be elucidated in the miniature ion thruster $\mu 1$; thus, the development of $\mu 1$ is currently dependent on some empirical designs. In order to clarify the mechanism of ECR discharges in a small space and to provide clear guidelines for optimum designs of $\mu 1$, numerical simulations could represent a powerful tool to compensate for lack of information obtained from experiments. Hence, we have been developing and improving a three-dimensional numerical model, which consists of a particle-in-cell simulation with a Monte Carlo collision algorithm (PIC-MCC) for the kinetics of charged particles,^{3,4} a finite-difference time-domain (FDTD) algorithm for the electromagnetic fields of 4.2-GHz microwaves⁵ and a finite element analysis for the magnetostatic fields of permanent magnets.

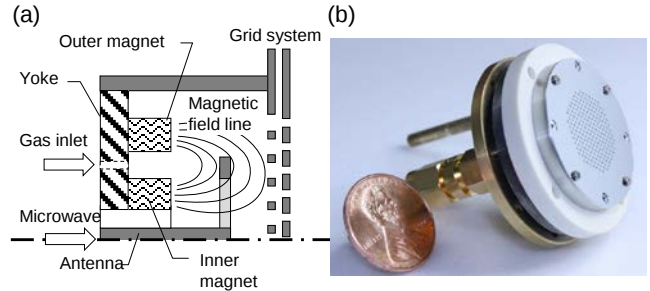


Figure 1. (a) Schematic diagram and (b) photograph image of the microwave discharge ion thruster $\mu 1$.

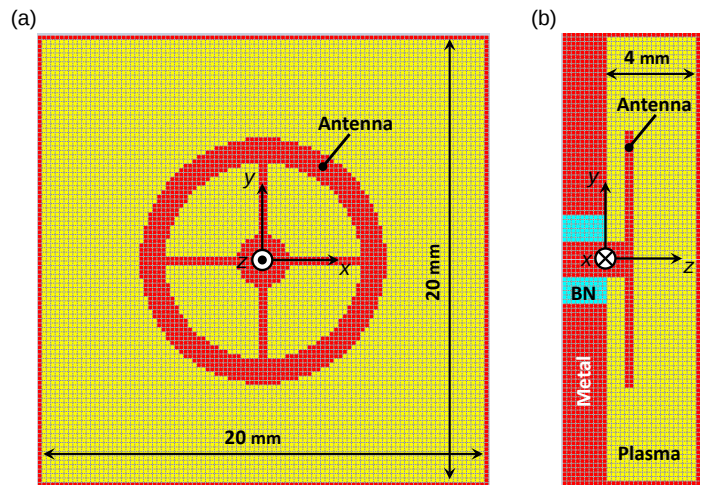


Figure 2. Computational grids for the calculation of $\mu 1$. (a) x-y plane and (b) y-z plane.

The calculation results are compared with experimental results taken from the $\mu 1$ visualized model in order to validate our numerical model.

II. Numerical Model

A. Configuration

Figure 2 shows the computational domain and grids of $\mu 1$ in this study. Cartesian coordinate system is employed and its origin is placed on the center of the antenna at the interface between the metal wall and the plasma in z direction. Both lengths in the x and y directions are set at 20 mm and the length in the z direction is 4 mm. The transverse electromagnetic (TEM) waves are injected into the system at the excitation plane ($z = -1.2$ mm) of the coaxial waveguide, where the inside of it is filled with the dielectric of boron nitride (BN). The microwave power is fed to the ring antenna through the four spokes as shown in Fig. 2(a). It should be noted that the BN region is also included in the electromagnetic-field calculation of microwaves, although the simulation area for charged particles is only the plasma region. The grid spacing is set at 0.2 mm at regular intervals. The space between inner and outer ring magnets is neglected and filled with metal for simplicity.

B. Assumption

- 1) Only Xe ions and electrons are treated as particles, and the ion species of interest is singly-ionized Xe^+ only.
- 2) Neutral particles are spatially uniform throughout the simulation and have Maxwellian velocity distribution at a gas temperature of 300 K ($= 0.026$ eV).
- 3) The reactions taken into account are elastic scattering, excitation, and ionization for electrons, and elastic scattering and charge exchange for ions, as below.
 - a. $e + \text{Xe} \rightarrow e + \text{Xe}$ (Elastic Scattering)
 - b. $e + \text{Xe} \rightarrow e + \text{Xe}^*$ (Excitation)
 - c. $e + \text{Xe} \rightarrow e + \text{Xe}^+ + e$ (Ionization)
 - d. $\text{Xe}^+ + \text{Xe} \rightarrow \text{Xe} + \text{Xe}^+$ (Charge Exchange)
 - e. $\text{Xe}^+ + \text{Xe} \rightarrow \text{Xe}^+ + \text{Xe}$ (Elastic Scattering)
- 4) The motion of excited-state atoms is not considered.
- 5) Coulomb collisions are not taken into account.
- 6) The magnetic fields of microwaves are neglected compared with the magnetostatic fields of the permanent magnets.
- 7) Since we have conducted calculations for a low power of microwaves at this stage, the plasma current is assumed to be neglected. The electromagnetic fields of microwaves and the electrostatic fields due to the space charge of charged particles are solved separately, and therefore self-consistent electromagnetic fields are not obtained strictly.

C. Electrostatic Field

The electrostatic field $\mathbf{E}_{\text{ES}}$ is given by

$$\mathbf{E}_{\text{ES}} = -\nabla\phi. \quad (1)$$

The potential ϕ is derived from the space charge of charged particles. The Poisson equation is given by

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \phi(x, y, z) = -\frac{\rho(x, y, z)}{\epsilon_0}. \quad (2)$$

Equation (2) is solved by using the method of successive-over-relaxation (SOR) with boundary conditions of zero at all the walls. Once the potential is obtained, the electrostatic field is determined by the central difference from the potential. It should be noted that we apply a digital smoothing algorithm to the space charge in order to decrease the numerical noise owing to the limited number of superparticles.⁶

D. Electromagnetic Field

The electromagnetic fields $\mathbf{E}_{\text{EM}}$ of microwaves are obtained by solving Maxwell's equations [Eqs. (3) and (4)] using FDTD approximation.

$$\nabla \times \mathbf{E}_{\text{EM}} = -\frac{\partial \mathbf{B}}{\partial t}, \quad (3)$$

$$\nabla \times \mathbf{B} = \mu_0 \left(\mathbf{j} + \varepsilon_r \varepsilon_0 \frac{\partial \mathbf{E}_{EM}}{\partial t} \right), \quad (4)$$

where the relative permittivity ε_r is set at 1 in the plasma and 4.5 in the dielectric (boron nitride: BN). The electric field components normal to metal surfaces are set to be zero.

E. Motion and Collisions of Charged Particles

Using the electrostatic field and electromagnetic field obtained above, we move charged particles by integrating the equation of motion:

$$\frac{d\mathbf{v}}{dt} = \frac{q}{m} (\mathbf{E}_{ES} + \mathbf{E}_{EM} + \mathbf{v} \times \mathbf{B}_{st}), \quad (5)$$

where the electric fields is the sum of $\mathbf{E}_{ES}$ and $\mathbf{E}_{EM}$, and only the magnetostatic fields of the permanent magnets $\mathbf{B}_{st}$ is taken into account because the magnetic fields of microwaves $\mathbf{B}$ is negligibly small compared with $\mathbf{B}_{st}$. The magnetostatic fields are determined with ANSYS EmagTM software, and the result is shown in Fig. 3, where the strength of the magnetic field $|\mathbf{B}_{st}|$ and the magnetic field lines are plotted, together with the thick lines in red representing the resonant magnetic field of 0.15 T for 4.2-GHz microwaves. Equation (5) is solved by Buneman-Boris method,⁷ and motion and collisions of charged particles can be treated separately by the principle of decoupling if a chosen time step gives a small collision probability.⁸ To reduce the cost of calculation time, we employ the null-collision method⁹ in MCC with cross sections for electrons¹⁰⁻¹² and ions.¹³ The postcollision velocities of electrons and ions are determined by the use of the conservation equations for momentum and energy.⁸

F. Numerical Procedures

First, the electromagnetic fields of microwaves injected are calculated with a time increment $\Delta t_{EM} = 2.98 \times 10^{-13}$ s (1/800 of a microwave cycle for 4.2 GHz) for a time span of typically several microwave periods to obtain a steady state of the electromagnetic fields without plasma. Second, PIC-MCC calculations are performed with a time step $\Delta t_e = 5.95 \times 10^{-12}$ s (1/40 of a microwave cycle) by using the time-varying electric field of $\mathbf{E}_{EM}(t) = |\mathbf{E}_{EM}| \cos(2\pi ft)$. Here, the motion of ions is updated with a time step $\Delta t_i = 2.38 \times 10^{-10}$ s (one microwave cycle) by neglecting $\mathbf{E}_{EM}$ and using the time-averaged $\mathbf{E}_{ES}$ because the frequency of 4.2 GHz is much higher than the ion plasma frequency. The time-averaged kinetic power deposition is recorded by calculating the change in kinetic energy of electrons and ions before and after each charged particle is moved on integrating the equation of motion.¹⁴ In the simulation, the power absorbed in the plasma P_{abs} is used as an input parameter. Last, we rescale the amplitude $|\mathbf{E}_{EM}|$ to yield the specified power absorbed in the plasma and iterate the above procedure until the steady state solution is obtained.

III. Numerical Results and Discussion

A Xe plasma discharge was calculated for $\mu 1$ shown in Fig. 2 under the base case condition, where the Xe gas pressure is $p = 1$ mTorr, the microwave frequency is $f = 4.2$ GHz, and the absorbed power is $P_{abs} = 0.3$ W. The initial densities of both electrons and ions are set at $1.0 \times 10^{16} \text{ m}^{-3}$ and distributed uniformly in the simulation area. The initial electron and ion temperatures are 2.0 and 0.05 eV, respectively. The macroscopic parameters, such as the electron density and electron temperature, shown below were determined by averaging over 50,000 microwave cycles (11.9 μ s) after the steady state was reached.

Figure 4 shows typical snapshots of the electric fields of microwaves at the x - y plane ($z = 2.0$ mm) and y - z plane ($x = 0.0$ mm), taken at the time when the electric fields reach the maximal values in a microwave period. The figure indicates the peak electric field near the circumference of the microwave antenna, especially between the antenna and the permanent magnets. The electric field in the z direction E_z is larger than the other components of the electric fields. The electric field in the x direction E_x is zero at $x = 0$ plane because of the symmetry, and thus E_z is dominant on the right side of the ring antenna at the y - z plane with $x = 0$ mm. As shown in Fig. 3, the magnetic field in the y direction B_y around ring antenna (between $y = 4$ mm and $y = 6$ mm) is dominant. These results indicate that electrons can be effectively heated in the ECR layer on the right side of the ring antenna.

Figure 5 shows an example of the electron trajectory near the ECR layer. The electron moves along the magnetic field line and travels back and forth as a result of the confinement due to the mirror magnetic fields; the electron gains the energy from microwaves during this motion because of the ECR. Moreover, the grad-B and/or curvature drift is also confirmed in Fig. 5(c). The energy of electrons can be high enough to exceed the threshold energy of the ionization (12.1 eV) owing to heating in the ECR layer, and therefore ring-shaped plasma discharges are expected to be generated and maintained in front of the ring antenna.

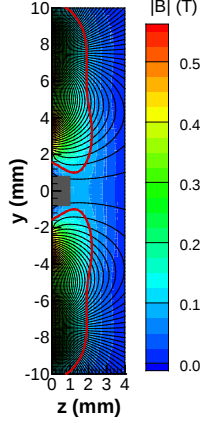


Figure 3. Contour plots of the strength of the magnetic field and the magnetic field lines.

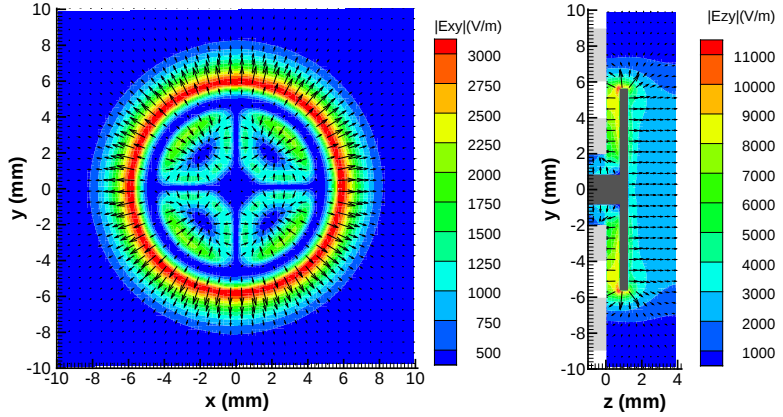


Figure 4. Typical snapshots of the electric fields of microwaves at the x-y plane ($z = 2.0$ mm) and y-z plane ($x = 0.0$ mm), taken at the time when the electric fields reach the maximal values in a microwave period.

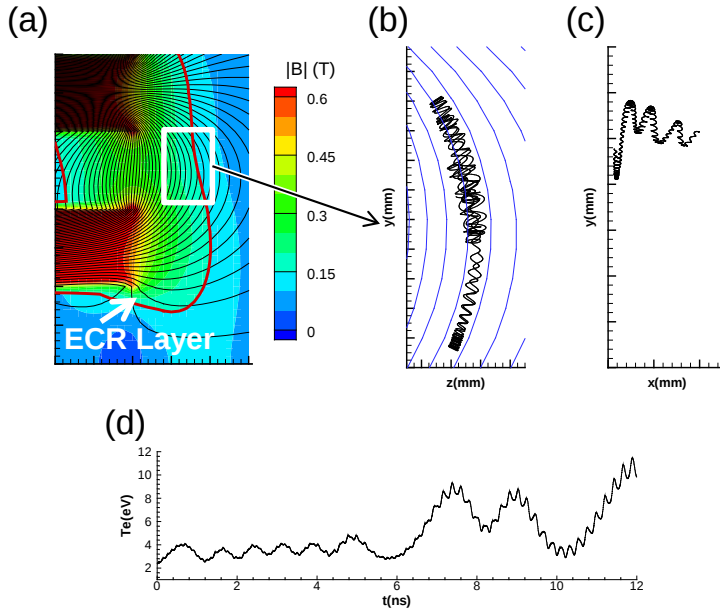


Figure 5. (a) Contour plots of the magnetostatic field, (b) trajectory of an electron at y-z plane in the white box depicted in (a) with magnetic field lines (blue thin line), (c) trajectory of an electron at x-y plane, and (d) the electron energy as a function of time.



Figure 6. Photograph image at the x-y plane of $\mu 1$ in plasma-discharging operation.

density, respectively. As shown in these figures, the peak plasma density is located in the ECR layer on the right side of the antenna, where the maximal value of the plasma density is $1.6 \times 10^{17} \text{ m}^{-3}$, and their distributions spread along the magnetic field lines. This result indicates that the plasma is well confined because of the mirror magnetic fields. The distribution of the electron density is almost the same as that of the ion density, indicating that quasi-neutrality is confirmed. The distribution of the plasma density obtained in the calculation is quite similar to that of the plasma discharge of $\mu 1$ in operation as shown in Fig. 6. The asymmetry of the distribution displayed around the center at x-y plane is probably due to the statistical fluctuation caused by a small number of superparticles, where the plasma density is less than a quarter of the peak density.

Figure 9 shows the three-dimensional distributions of the time-averaged electron temperature, where the electron temperature is defined by the following equation with the number of superparticles N .

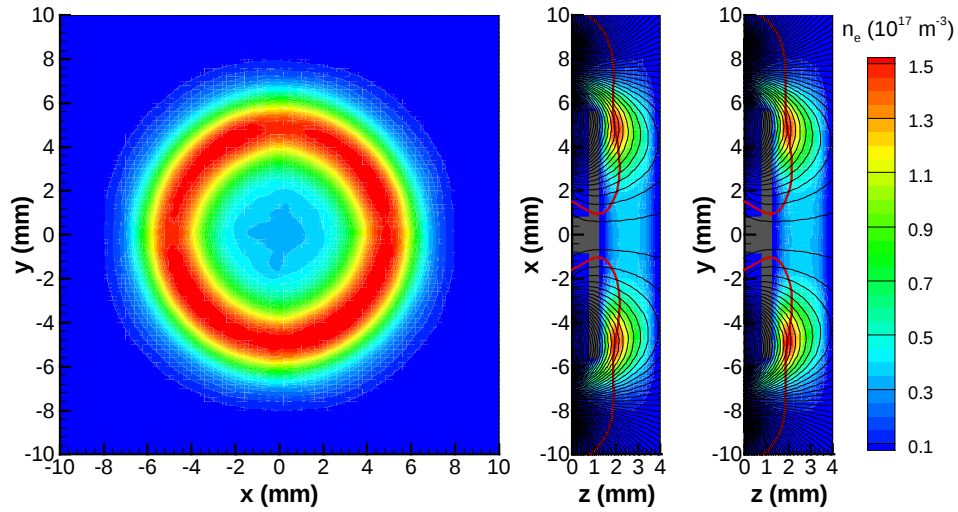


Figure 7. Contours of the electron density with magnetic field lines (black) and ECR layer (red line).

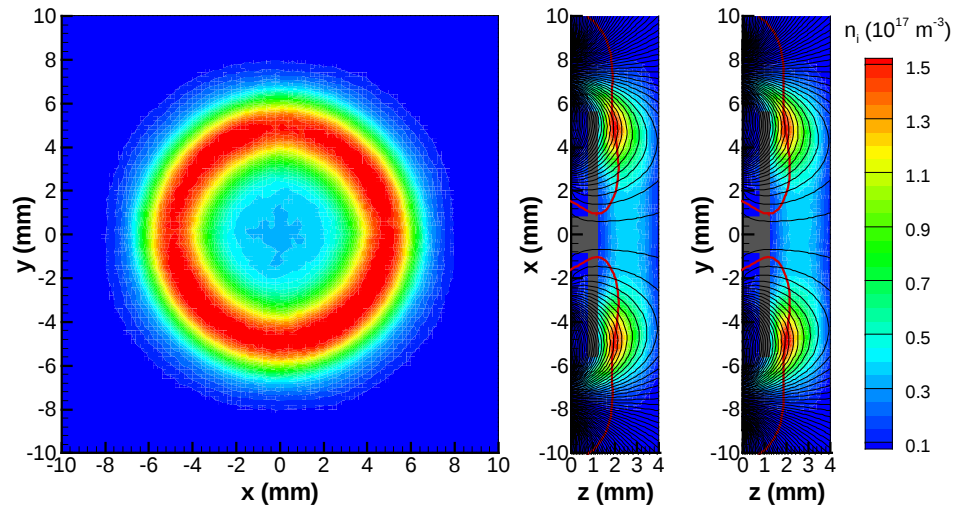


Figure 8. Contours of the ion density with magnetic field lines (black) and ECR layer (red line).

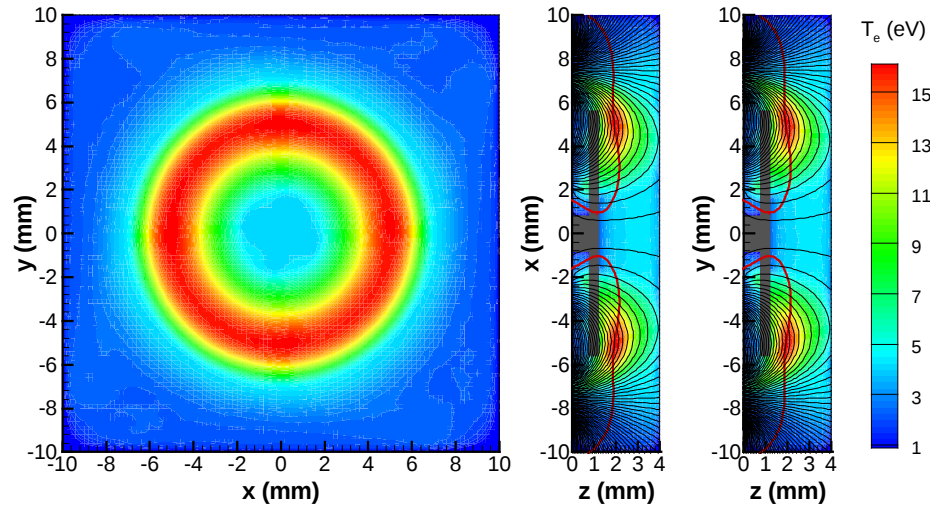


Figure 9. Contours of the electron temperature with magnetic field lines (black) and ECR layer (red line).

$$T_e = \frac{N}{3(N-1)} \frac{m}{q} \left(\frac{1}{N} \sum v^2 - \left(\frac{1}{N} \sum v \right)^2 \right). \quad (6)$$

The distribution of the electron temperature is almost the same as that of the plasma density, where the peak electron temperature obtained is 16 eV. The electron temperature in front of the ring antenna is much larger than the ionization energy of Xe. Since the temperature defined by Eq. (6) is just a macroscopic parameter, a large population of high-energy electrons is expected, which is described below. The three-dimensional distributions of the time-averaged potential are also shown in Fig. 10, where the peak plasma potential obtained is 21 V. The potential has a little broad peak compared with the plasma density and the electron temperature owing to the diffusion characteristic of Eq. (2).

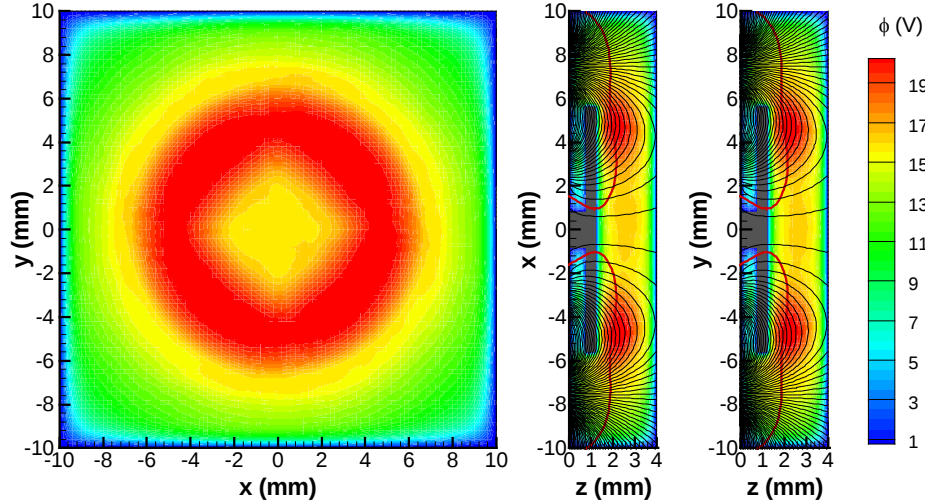


Figure 10. Contours of the potential with magnetic field lines (black) and ECR layer (red line).

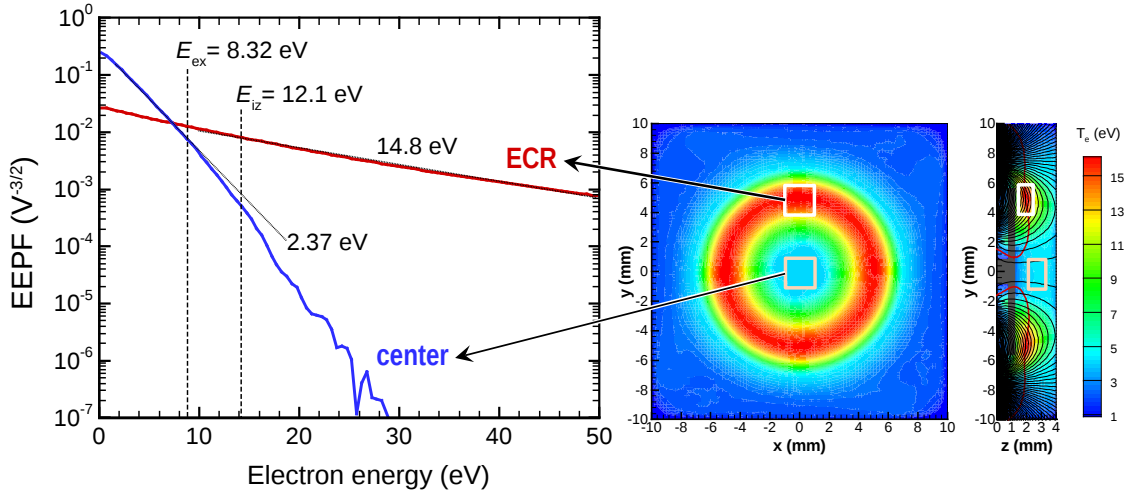


Figure 11. Normalized EEPF at the center of the x-y plane and in the ECR layer.

Figure 11 shows the normalized electron energy probability function (EEPF) at the center of the x-y plane and in the ECR layer. As shown in the figure, depletion of EEPF is clearly seen at the center owing to the inelastic collision loss and almost no power absorption from microwaves. However, the ECR produces a large number of high-energy electrons, resulting in a high degree of ionization in the ECR layer. This large difference in EEPFs at different points leads to the plasma distribution shown above.

Figures 12 and 13 indicate the three-dimensional distributions of the time-averaged ionization rate and excitation rate, respectively. Since the threshold energy of ionization is higher than that of excitation and the cross section of the ionization is larger than that of excitation at higher electron energy (> 22 eV), the maximal value of the ionization rate is larger than that of the excitation rate and the distribution of the ionization rate is more localized in

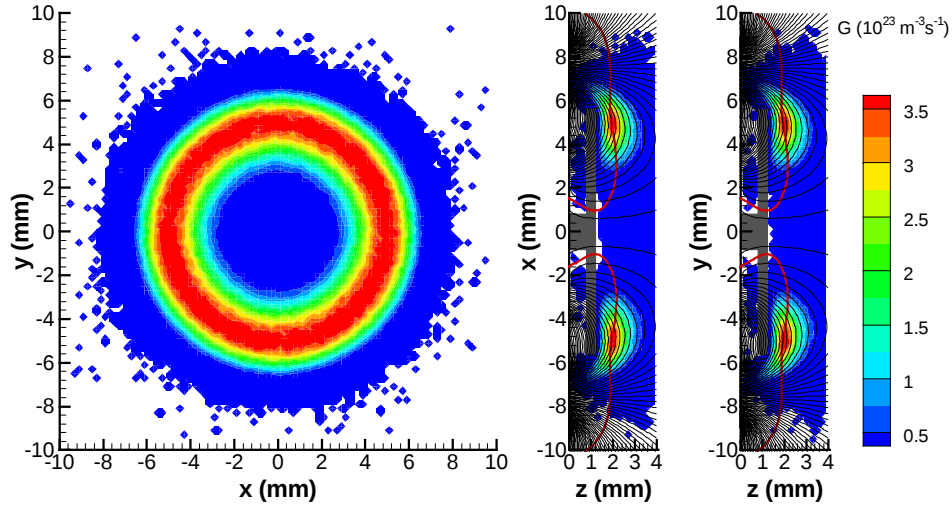


Figure 12. Contours of the ionization rate with magnetic field lines (black) and ECR layer (red line).

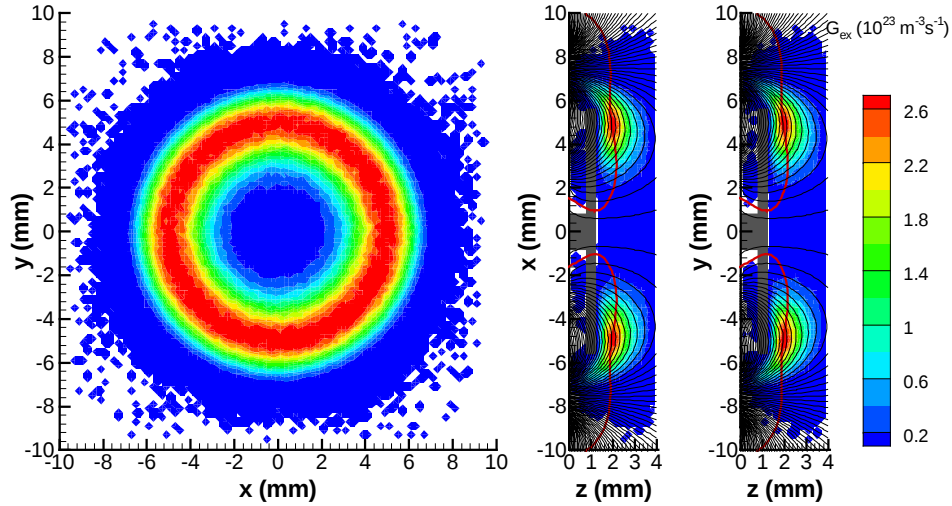


Figure 13. Contours of the excitation rate with magnetic field lines (black) and ECR layer (red line).

the ECR layer. The excitation rate is distributed a little more broadly. It should be noted that their values equal to or less than zero are not plotted for visibility.

Table 1 summarizes power balance results. The total power absorbed by the plasma P_{abs} is due to the electron heating P_e and ion heating P_i , whereas the total power lost by the plasma P_{loss} is equal to the sum of the power loss of electron and ion to the walls ($P_{e,\text{wall}}$ and $P_{i,\text{wall}}$), and collisions with neutral particles. Here the collision losses are elastic scattering, excitation, and ionization for electrons ($P_{e,\text{elas}}$, $P_{e,\text{exc}}$, and $P_{e,\text{ion}}$), and elastic scattering and charge exchange for ions ($P_{i,\text{elas}}$ and $P_{i,\text{cex}}$). Most of the power absorption occurs in the electron motion. However, significant ion energy deposition can also be seen, especially in the z direction, where a large area of the wall exists just downstream of the ring antenna with a small gap. The ions are accelerated through the sheath potential drop and lose their energy on the wall. Although the electrons also lose their energy on the wall significantly because of the small area, the power dissipation of ionization is much larger than

Table 1. Power balance.

P_{abs} (mW)	300	P_{loss} (mW)	300
$P_{e,x}$	57.4	$P_{e,\text{wall}}$	83.2
$P_{e,y}$	57.6	$P_{i,\text{wall}}$	111
$P_{e,z}$	73.1	$P_{e,\text{elas}}$	0.0
$P_{i,x}$	11.1	$P_{e,\text{exc}}$	39.0
$P_{i,y}$	11.0	$P_{e,\text{ion}}$	65.8
$P_{i,z}$	89.9	$P_{i,\text{elas}}$	0.2
		$P_{i,\text{cex}}$	0.9

that of excitation. This result is consistent with the results shown in Figs. 12 and 13. The power absorbed by the plasma P_{abs} and the power lost by the plasma P_{loss} agree to within 1%. We also see similar good agreement between P_e and $P_{\text{loss},e}$ and between P_i and $P_{\text{loss},i}$.

IV. Comparison with Experimental Results

To validate our numerical model, the comparison with experimental results is required. However, owing to the small size of $\mu 1$ and strong magnetic fields inside the discharge chamber, probe diagnostics cannot be readily done. Hence, laser absorption spectroscopy (LAS) is a promising and useful technique for the sensitive and quantitative measurement of plasma particles. In this study, we measured the number density of Xe metastable state ($1s_5$), the lifetime of which is quite long (~ 40 s).

LAS experimental results are obtained from the $\mu 1$ visualized model as shown in Fig. 14. The measurement area was taken to be 3 mm in the z direction and 20 mm in the y direction, and the interval was set at 0.1 mm. The microwave power was 2 W and Xe gas flow rate was 0.15 sccm, which results in the Xe pressure of about 1 mTorr. The experimental setup and procedure are described elsewhere.^{15,16}

Whereas the LAS experiment produces the number density of Xe metastable, the PIC-MCC simulation determines charged particles only. However, the PIC-MCC also yields the excitation rate as shown in Fig. 13, which is

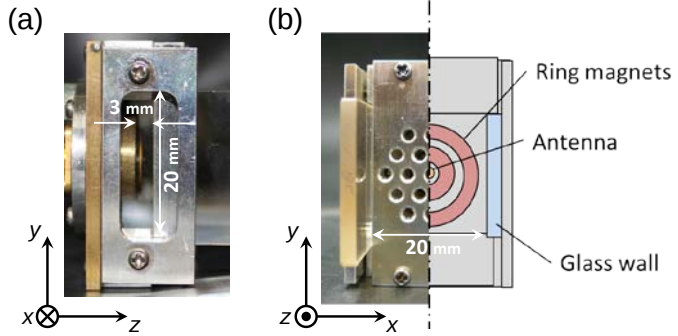


Figure 14. (a) Side (y - z plane) and (b) front (x - y plane) views of the $\mu 1$ visualized model.

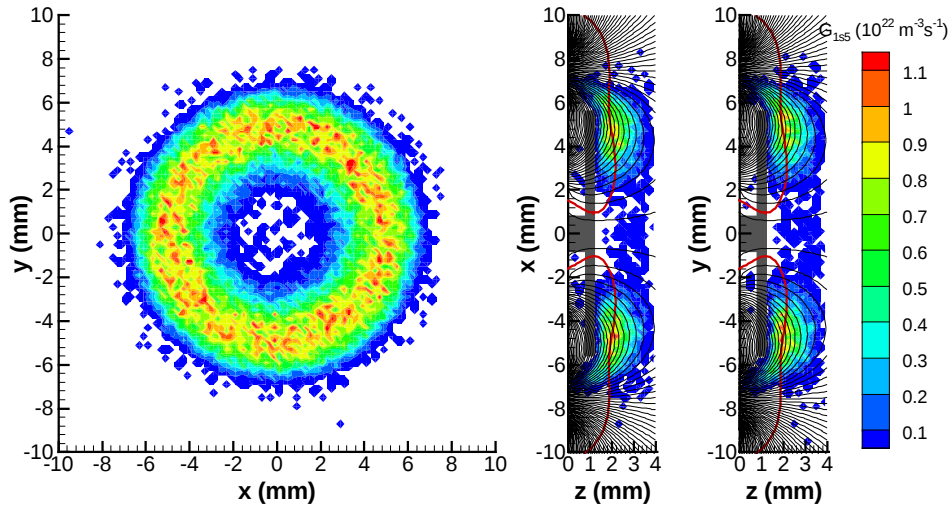


Figure 15. Contours of the excitation rate which leads to metastable $1s_5$ with magnetic field lines (black) and ECR layer (red line).

derived from the total excitation cross section. Using the excitation rate in Fig. 13 would lead to an overestimation of Xe metastable of $1s_5$. Therefore, we take into consideration the cross section which is related to $1s_5$ only. It should be noted that the transitions $2p_{10-6}$ to $1s_5$ are also taken into account.¹⁷ The three-dimensional distributions of the time-averaged excitation rate of $1s_5$ are shown in Fig. 15. The excitation rate of $1s_5$ is less than the total excitation rate by more than one order of magnitude. The distribution of $1s_5$ is derived from the excitation rate in Fig. 15 on the assumption that Xe metastable of $1s_5$ has Maxwellian velocity distribution at a temperature of 300 K, there are no collisions between $1s_5$ and the other particles, and $1s_5$ disappears when it reaches the walls and antenna.

Figure 16 shows the two-dimensional distributions of the time-averaged $1s_5$ obtained from the calculation and the LAS experiment. The distributions of $1s_5$ are similar to each other. If the density of $1s_5$ is proportional to the microwave power, the numerical result would be in reasonable agreement with the experimental result. Even though

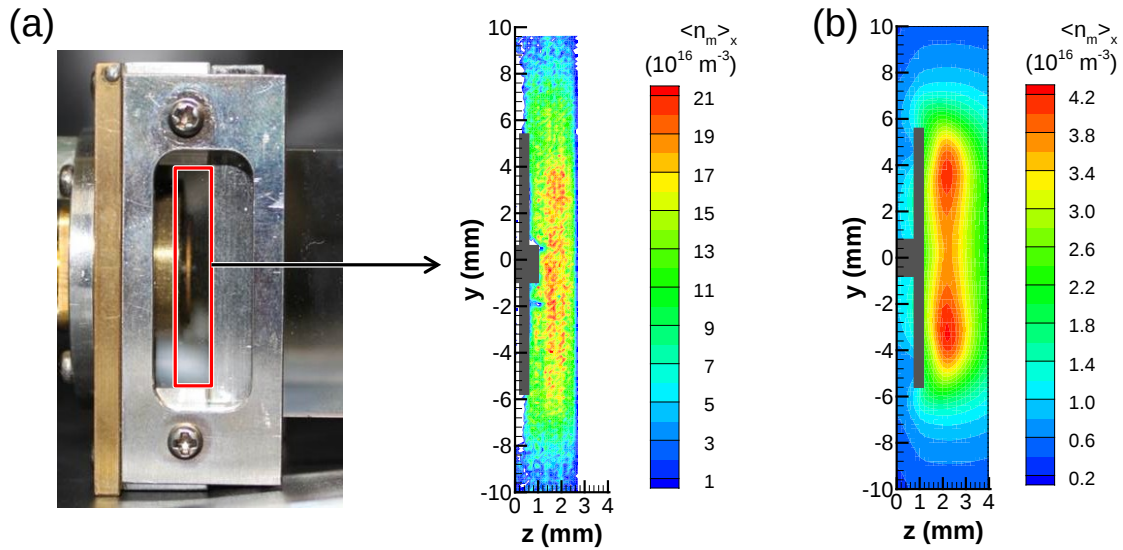


Figure 16. Contours of the metastable $1s_5$ (a) obtained from the experiment and (b) from the calculation.

the plasma current is not fed back to the Maxwell equations, our numerical PIC-MCC model could reproduce the experimental results.

V. Conclusion

In the present work, we have developed a numerical model for a miniature microwave discharge ion thruster $\mu 1$ to elucidate the mechanism of ECR discharges confined in a small space. Simulation results have shown that the electrons are well confined owing to the mirror magnetic fields and can be effectively heated in the ECR layer downstream of the ring antenna because of the configuration of the magnetostatic fields and microwave electric fields. The distribution of the plasma density obtained in the calculation is quite similar to that of the plasma discharge of $\mu 1$ in operation. Moreover, the distribution of Xe metastable of $1s_5$ is also compared with the experimental result. Even though our model can simulate plasma discharges at very low power only, the numerical results reasonably reproduce the experimental results. In future work, the plasma current is also taken into account in our model and plasma characteristics at nominal power range will be calculated.

Acknowledgments

This work was financially supported in part by a Grant-in-Aid for Scientific Research (B) (Grant No. 25289304) from the Japan Society for the Promotion of Science.

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