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Study of energy relaxation processes of the surface produced negative ions by using the 3D3V PIC simulation

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Contents

Introduction (I)

- A negative ion source which can produce negative ion beams with high power and long pulse is the key component for the negative ion based NBI system for plasma heating and current drive of magnetic fusion reactors.

- For the design and development of such a negative ion source, the study of the H^- ion beam optics is one of the crucial issues since the H^- ion beams with poor beam optics will cause the excessive heat loads and the breakdown in the accelerator.

- In the present tandem-type negative ion sources, surface production is dominant for the H^- ion production process. In surface production, the H^+ ions and/or H atoms impinge on the PG surface with the low work function, and are converted to H^- ions. Since the H atoms are generated mainly by dissociation of the H_2 molecules of the Frank-Condon process, or the H^+ ions are accelerated through the sheath, these incident H atoms and/or H^+ ions are considered to have the energy of a few eV.

Introduction (II)

- From particle simulations and semi-empirical formulas, the energy reflection coefficient for the low energy of a few eV is estimated to be around 0.5. Therefore, the surface produced H^- ions are considered to be launched with the initial energy of 1 ~ 2 eV.

- However, it is well-known that negative ion beams in the tandem-type negative ion source have good beam optics. From the measured emittance of the H^- ion beam, one can estimate the H^- ion temperature to be 0.1 eV of the order of the magnitude, and it is reported that the measured H^- ion temperature is 0.1 eV.

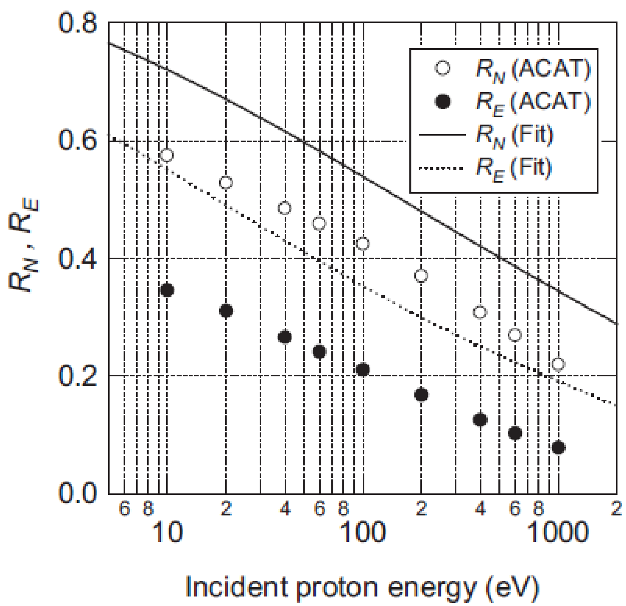


FIGURE 6. Comparison of R_N and R_E calculated by ACAT code to those obtained from empirical formulas introduced in reference [14].

M. Wada, M. Bacal, T. Kasuya, S. Kato, T. Kenmotsu and M. Sasao, *AIP conference proceedings*, **1515**, 59-65 (2013).

Introduction (III)

・The energy relaxation of H^- ions is possible reason for the good beam optics of the surface produced H^- ions.

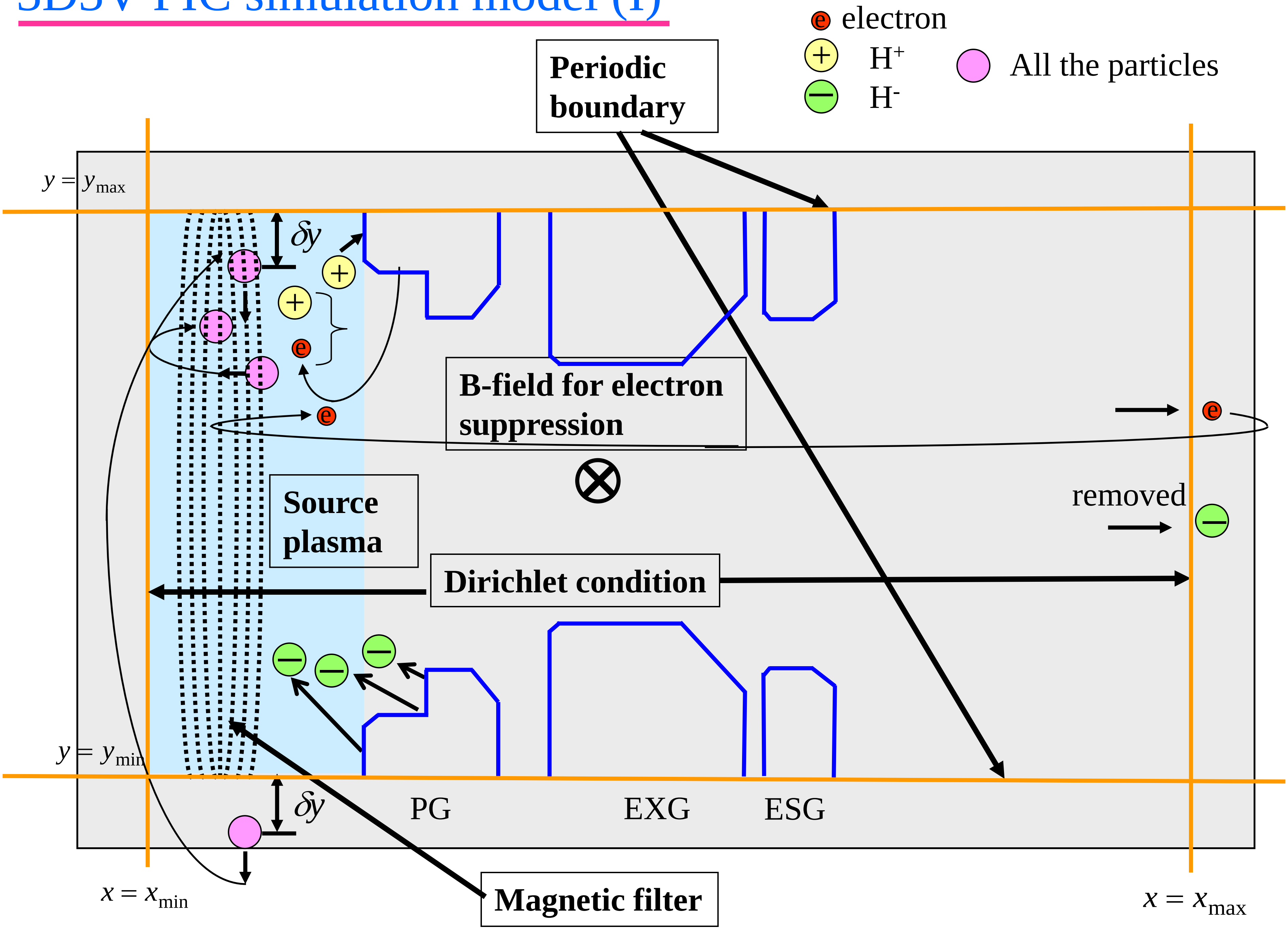
・The previous studies by using a three-dimensional Monte Carlo simulation show that the Coulomb collision with the H^+ ions and the charge exchange collision with the H atoms ($H^- + H \rightarrow H + H^-$) contribute to the energy relaxation of H^- ions. However, the background plasma is not solved self-consistently. Moreover, the electric field for the H^- extraction has not been taken into account.

・Recently, the study of the H^- energy relaxation due to the Coulomb collision has been carried out by using the 2D3V PIC simulation[1]. Since the PIC simulation can solve the plasma and the electric field self-consistently, it is useful to clarify the physical mechanism of H^- ion extraction and beam optics.

・In this study, we extend to the 3D3V PIC simulation model, and verify the energy relaxation processes in detail. Moreover, the effect of the energy relaxation processes on the H^- ion beam optics is investigated.

1. I. Goto, K. Miyamoto, S. Nishioka, S. Mattei, J. Lettry, S. Abe, and A. Hatayama, *Rev. Sci. Instrum.*, **87** 02B918/1-3 (2016).

3D3V PIC simulation model (I)



3D3V PIC simulation model (II)

Main physical parameters in the source region

Physical parameters	Symbol	Value
Electron temperature	T_e	1 eV
Hydrogen ion temperature	T_{H+} T_{H-}	0.25 eV 0.25 eV (volume production) 1.50 eV (surface production)
Electron density	n_e	10^{18}m^{-3}
Electron Debye length	λ_{De}	7.4×10^{-6} m
Electron plasma frequency	ω_{pe}	5.6×10^{10} rad/s

- Initial number of super-particles : 10^7 of the order of the magnitude
- The number of numerical grid is 433 × 153 × 153 in the *x*, *y* and *z* directions respectively, which corresponds to 54 mm × 19 mm × 19 mm in real size.
- Electrons, H^+ ions, and volume produced H^- ions are assumed to be launched with Maxwellian distributions. The surface produced H^- ions are assumed to be launched with half-Maxwellian distribution.

3D3V PIC simulation model (III)

・The following collision processes are taken into account as the energy relaxation processes of H^- ions.

1) Coulomb collision
A binary collision model by the Monte Carlo method is used.

2) Charge exchange collision (H^- (fast) + H (slow) $\rightarrow$ H^- (slow) + H (fast))
The null collision model is used.

$n_{H2} = 1.88 \times 10^{19}$ m^{-3} ($p_{H2} = n_{H2}\, k\, T_{H2}$, p_{H2} = 0.3 Pa, T_{H2} = 0.1 eV)

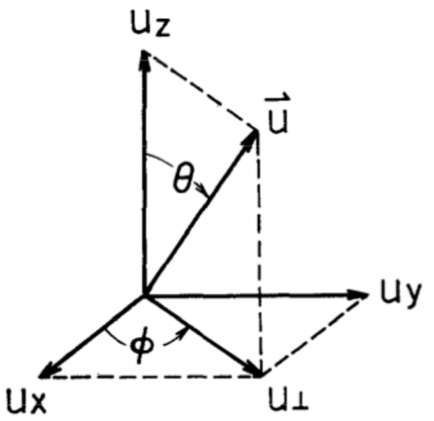
$n_H/n_{H2} = 0.5$ (U. Fantz, et al., *Rev. Sci. Instrum.*, **77**, 03A516 (2006).)

$n_H = 9.38 \times 10^{19}$ m^{-3}

・In the present model, the mutual neutralization ($H^- + H^+ \rightarrow H + H$) is taken into account as H^- ion destruction process.

Binary collision model by the Monte Carlo method

A binary collision model (BCM)[2] by the Monte Carlo method is applied to the Coulomb collision with the H^+ ions.



$$\Phi = 2\pi\delta_1 \qquad \langle \delta_2 \rangle = 0$$

$$\theta = 2\arctan\delta_2 \qquad \langle {\delta_2}^2 \rangle = \frac{n_L (e_1 e_2)^2 \ln\Lambda}{8\pi\varepsilon_0^2 m_{\alpha\beta} u^3}\Delta t$$

δ_1, δ_2 : uniform random number

n_L : particle density

$m_{\alpha\beta}$: reduced mass

$\ln\Lambda$: Coulomb logarithm

Δt : time step

$$\Delta u_x = \frac{u_x}{u_\perp} u_z \sin\theta\cos\Phi - \frac{u_y}{u_\perp} u \sin\theta\sin\Phi - u_x(1-\cos\theta)$$

$$\Delta u_y = \frac{u_y}{u_\perp} u_z \sin\theta\cos\Phi - \frac{u_x}{u_\perp} u \sin\theta\sin\Phi - u_y(1-\cos\theta)$$

$$\Delta u_z = -u_\perp \sin\theta\cos\Phi - u_z(1-\cos\theta)$$

$$u_\perp = \sqrt{u_x^2 + u_y^2}$$

2. T. Takizuka and H. Abe, J. Comput. Phys. **25**, 205-219 (1977).

Model of the charge exchange collision

- As for the charge exchange collision, an electron moves from the surface produced H^- ion (fast ions) to a slow H atom, which then leaves behind a slow scattered H^- ion.
- This slow H^- ion is scattered isotropically: the scattering angles are randomly chosen as

$$\theta = \pi U_1, \Phi = 2\pi U_2 \qquad (U_2, U_3\text{: a uniform random number})$$

- The speed of the scattered H^- ion is chosen to match the H atom velocity distribution (T_H = 0.1 eV).
- Whether the charge exchange collision occurs or not is determined by using the null collision model[3]. In the present model, the mutual neutralization ($H^- + H^+ \rightarrow H + H$) is taken into account other than the charge exchange collision.

$$R \le \upsilon_1(E_i)/\upsilon' \text{ (collision type 1)}$$

$$\upsilon_1(E_i)/\upsilon' < R \le (\upsilon_1 + \upsilon_2)/\upsilon' \text{ (collision type 2)}$$

$$\vdots$$

$$\sum_{j=1}^{N} \upsilon_j(E_i) \Big/ \upsilon' < R \text{ (null collision)}$$

E_i : energy of the particle i

$$\upsilon' = \max(n_T \sigma_T \nu)$$

$$\sigma_T = \sigma_1 + \cdots \sigma_N$$

υ_j collision frequency for the collision type j

R : uniform random number

3. V. Vahedi, M. Surendra, *Comput. Phys. Commun.*, **87**, 179-198 (1995).

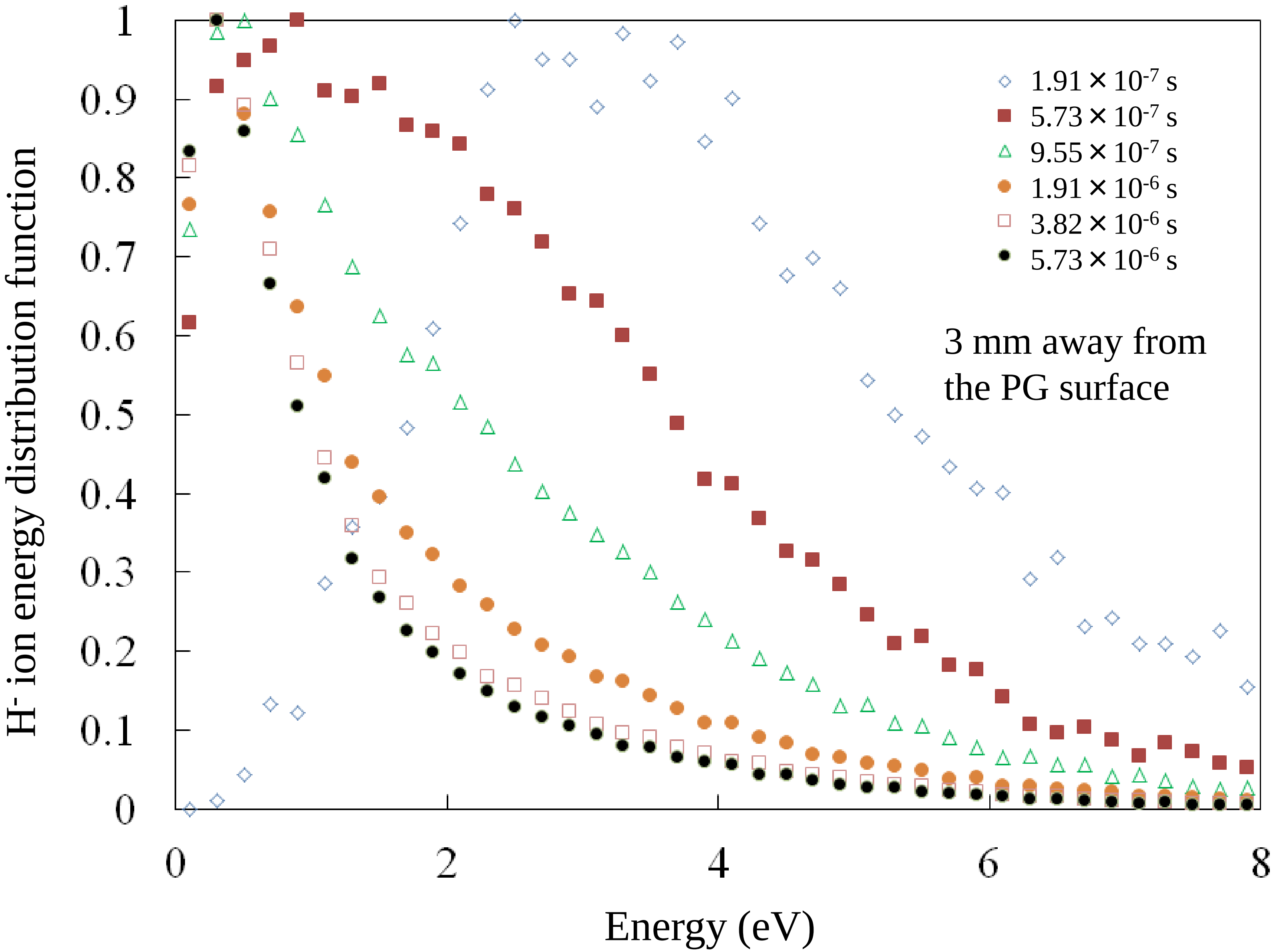
Analysis of energy relaxation processes of H^- ions

- Time evolutions of H^- ion energy and velocity distributions will be shown.
- The energy relaxation process is analysed without H^- ion extraction. Thus, the voltages of the PG, the EXG, the ESG, and the boundary of $x = x_{max}$ are set to be zero.
- Moreover, the volume produced negative ions are not included in this analysis.

Initial number of super-particles

electron: $N_e = 1.6 \times 10^7$, H^+: $N_{H+} = 1.6 \times 10^7$

Time evolution of the H^- ion energy distribution function with the Coulomb collision



Estimation of the characteristic time of the energy relaxation due to the Coulomb collision

The characteristic time of the energy relaxation due to the Coulomb collision is given by

$$\tau_{cc}^{e} = \frac{6\sqrt{3}\pi\varepsilon_0^2\sqrt{m_{H-}}\left(kT_{H-}\right)^{1.5}}{q^4 n_{H+}\ln\Lambda}.$$

By substituting n_{H+} = 1.0 × 10^{18} m^{-3}, T_{H-} = 1.5 eV into the above equation, τ_{cc}^{e} can be estimated to be 1.87 × 10^{-6} s.

Thus, the simulation result agrees well with this estimated characteristic time of the order of the magnitude.

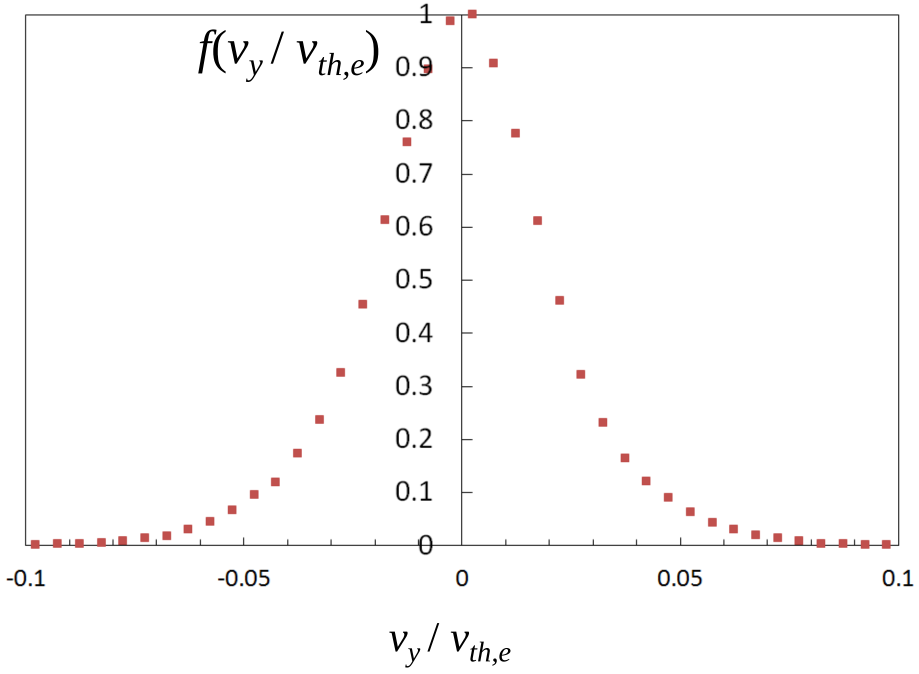
The H^- ion velocity distribution with the Coulomb collision

The H^- ion temperature is reduced to 0.61 eV from 1.5 eV due to the Coulomb collision.

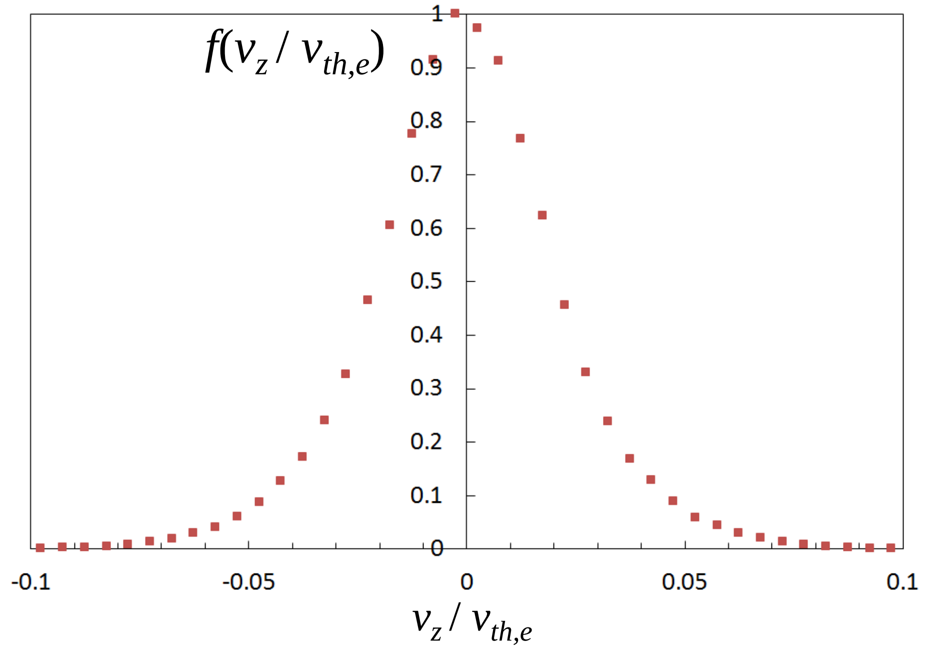
The H^- ion velocity distribution functions perpendicular to the direction of H^- extraction with the Coulomb collision

$v_{th,e}$: thermal velocity of electrons

(a) v_y

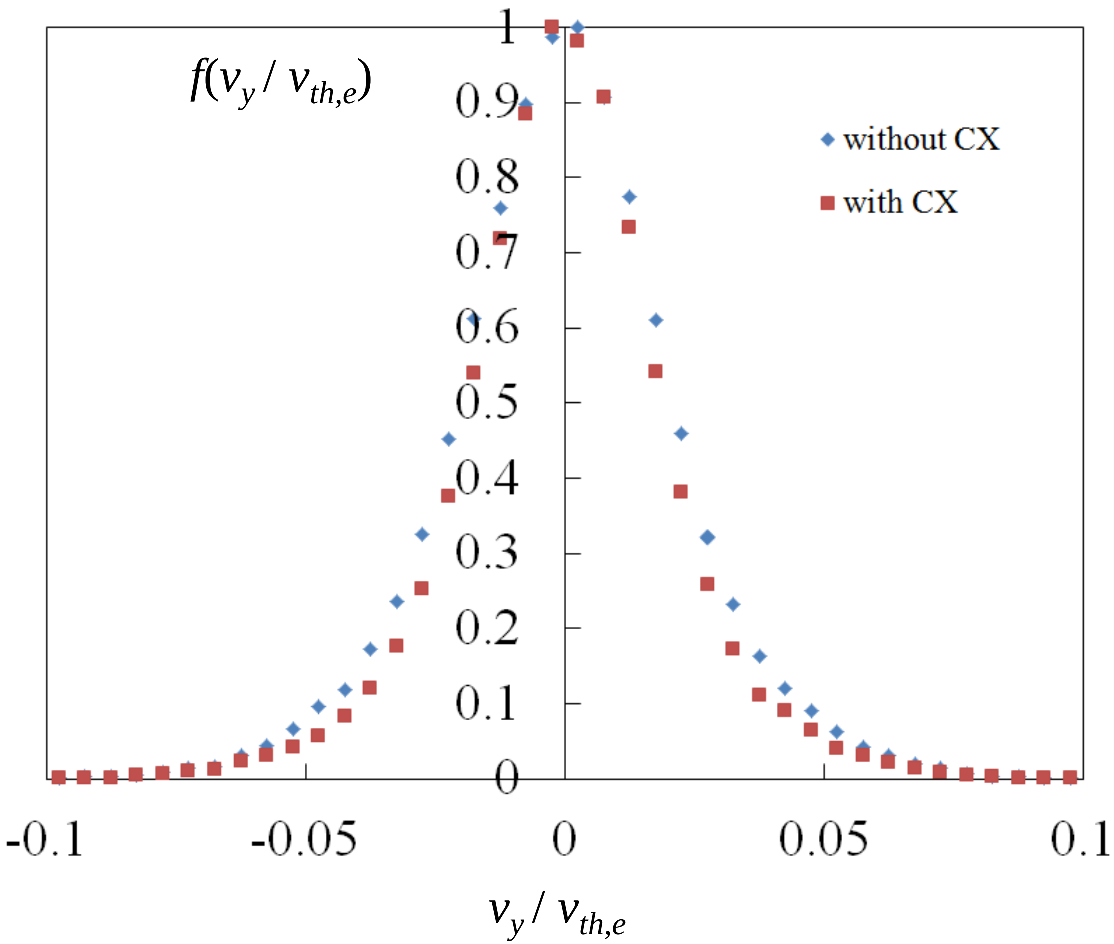


(b) v_z



Comparison of the H^- ion velocity distribution with and without the charge exchange (CX)

It is indicated that the Coulomb collision is dominant for the energy relaxation under the present calculation condition (n_e = 1.0 × 10^{18} m^{-3}, T_{H+} = 0.25 eV, n_H/n_{H2} =0.5, n_H = 9.4 × 10^{18} m^{-3}, T_H = 0.1 eV).



T_{H-} ∼ 0.61eV (without CX)
T_{H-} ∼ 0.49 eV (with CX)

At the energy of 1 eV, for example, each collision frequency is estimated to be

- Coulomb collision : 9.82 × 10^5 s^{-1}
- Charge exchange : 1.84 × 10^5 s^{-1}

Analysis of the effect of the energy relaxation processes on the H^- ion beam optics

- Emittance diagrams without and with the energy relaxation processes will be compared.

- The voltages of the PG, the EXG, the ESG, and the boundary of $x = x_{max}$ are applied. Each voltage corresponds to 0V (PG), 7.6 kV (EXG and ESG), and 52.4 kV (the boundary of $x = x_{max}$).

- Initial number of super-particles

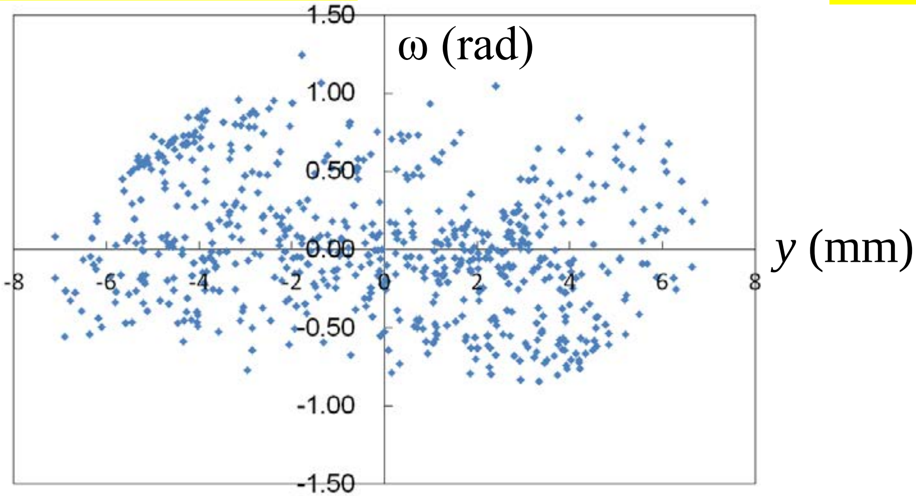
electron: $N_e = 2.96 \times 10^7$, H^+: $N_{H+} = 3.11 \times 10^7$, volume produced H^-: $N_{H-} = 1.56 \times 10^6$

- The H^- ion beam current densities are estimated as follows:

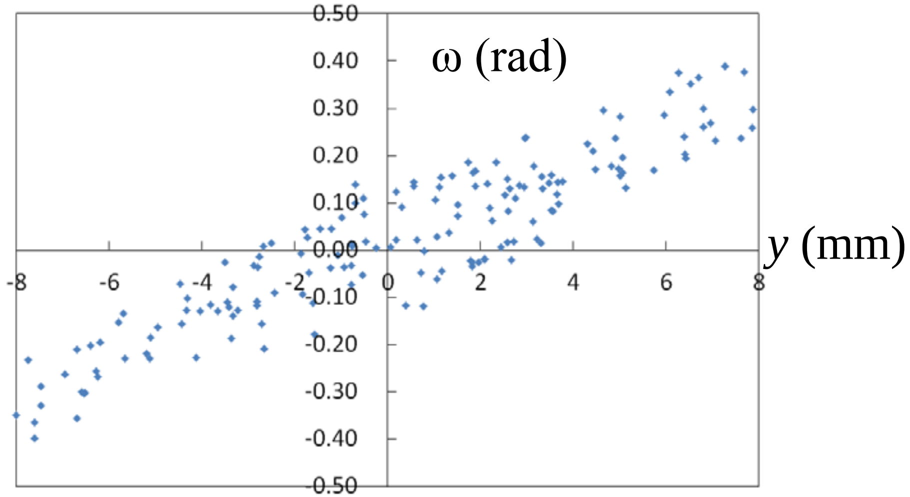
(i) Only volume produced H^- ions : 3 mA/cm^2
(ii) volume + surface produced H^- ions :
without the energy relaxation processes : 16 mA/cm^2
with the energy relaxation processes : 21 mA/cm^2

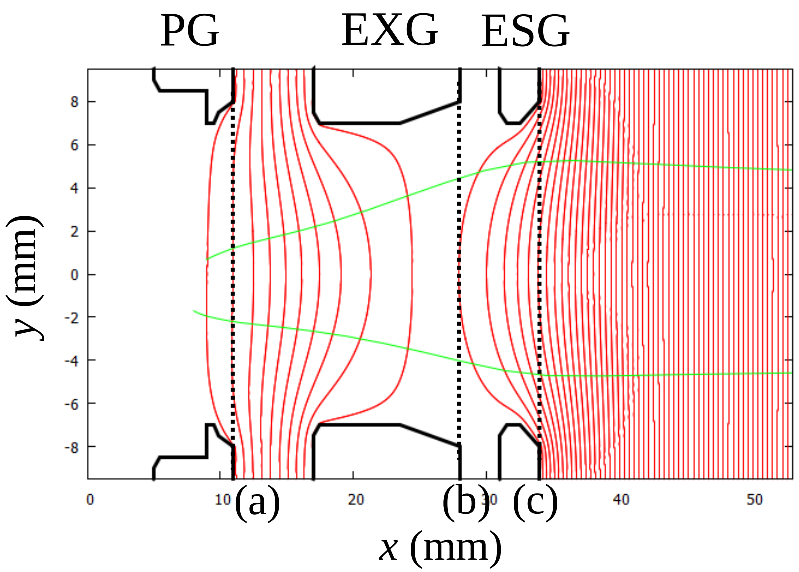
Emittance diagrams of H⁻ ions without energy relaxation

(a) Exit of the PG

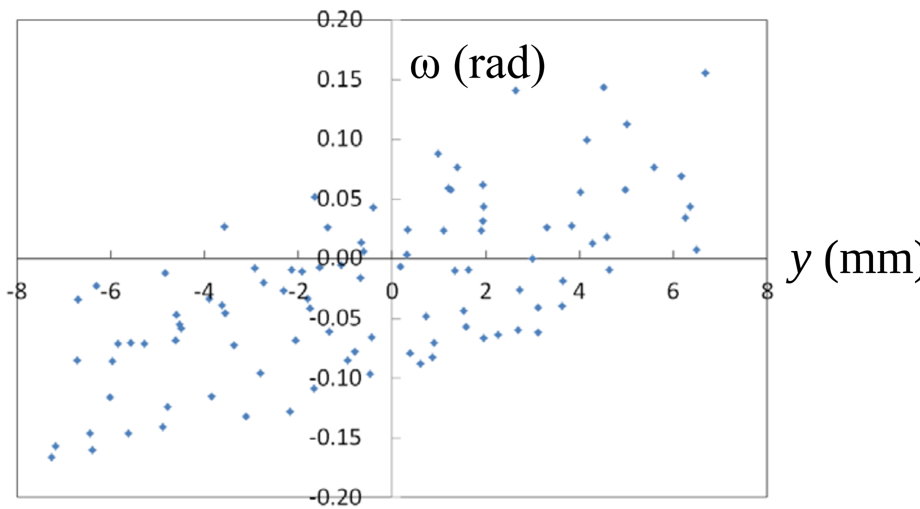


(b) Exit of the EXG





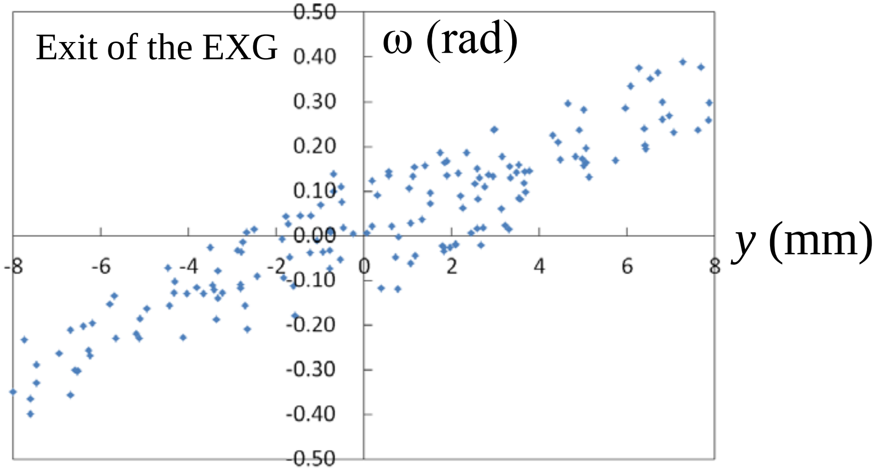
(c) Exit of the ESG

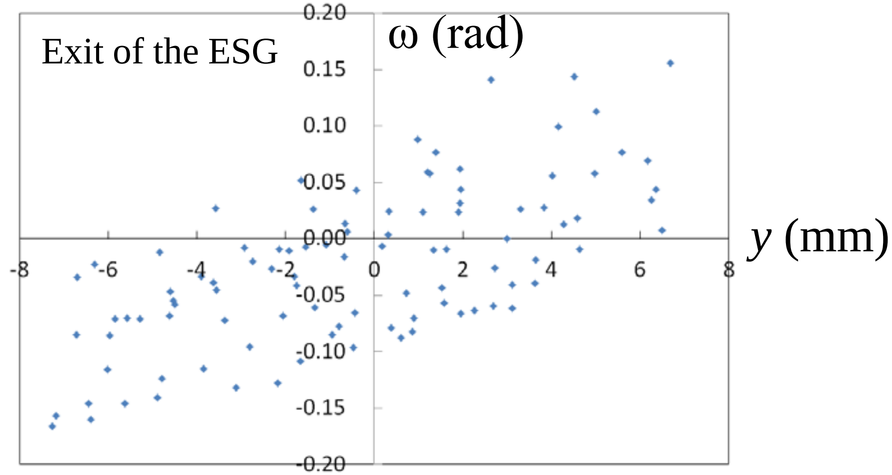


Comparison of emittance diagram of H^- (I)

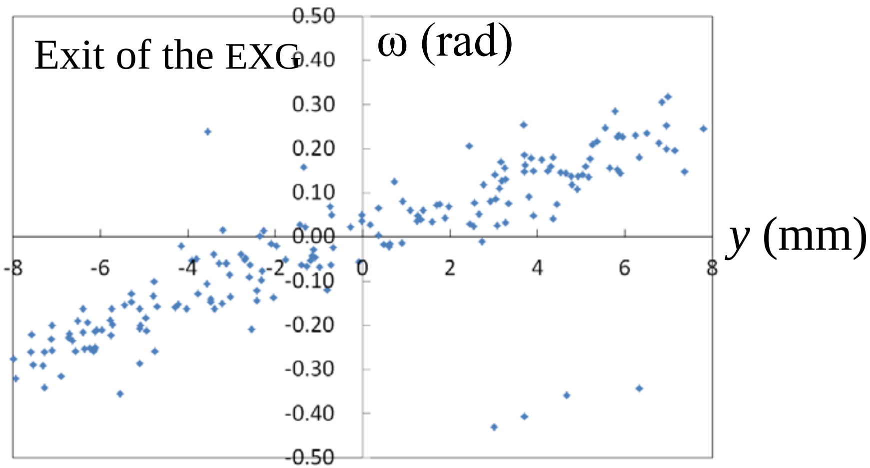
It is shown that the emittances with the energy relaxation processes are smaller than those without the energy relaxation processes.

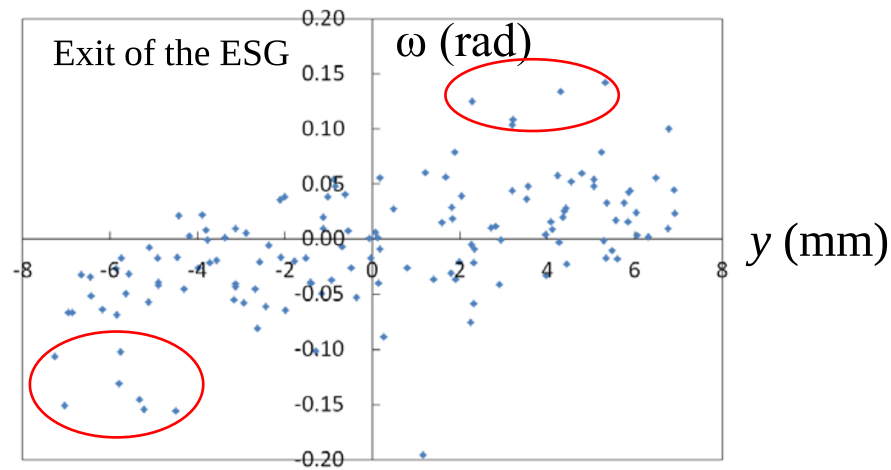
Without the energy relaxation processes





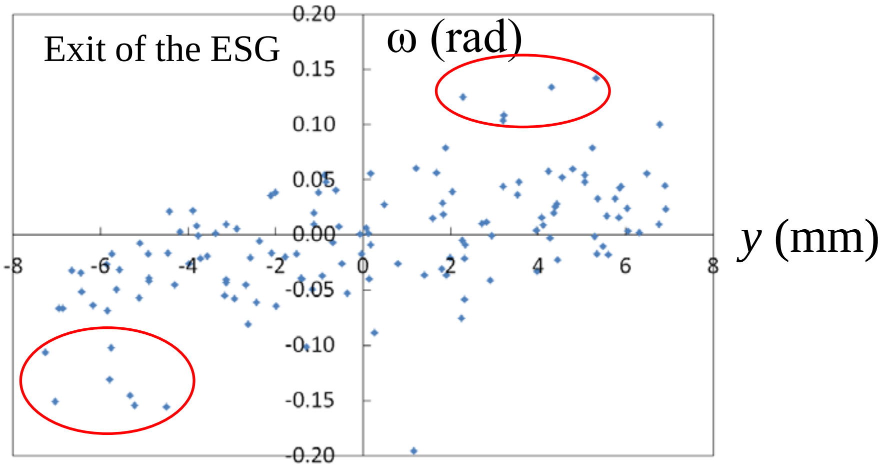
With the energy relaxation processes

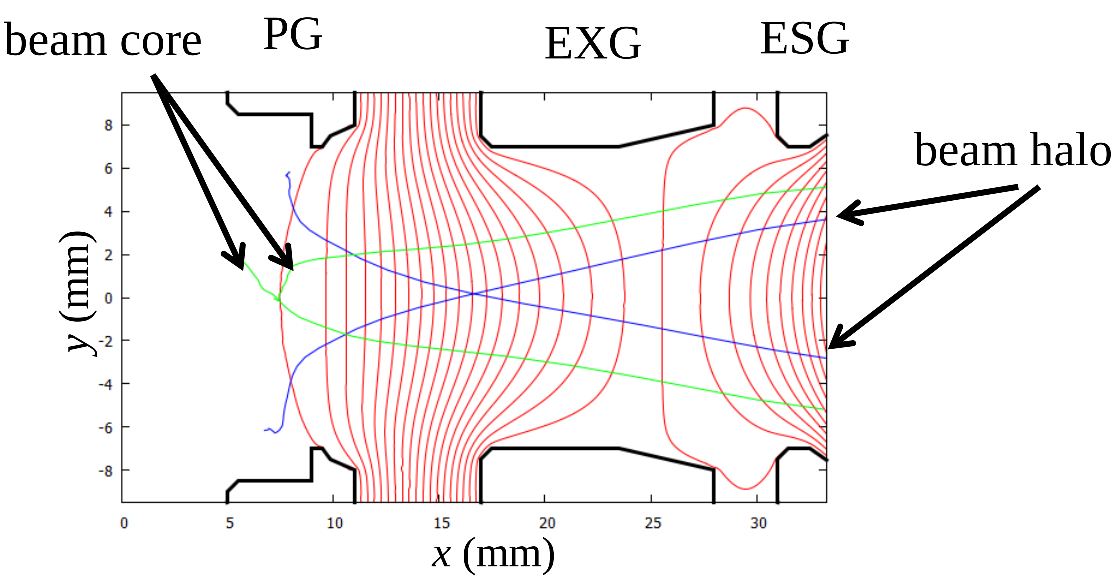




Comparison of emittance diagram of H^- (II)

It is indicated that the separation of the beam core and the beam halo in the emittance diagram becomes clearer with the energy relaxation processes.





Summary

We investigate the energy relaxation processes of H^- ions in a negative ion source, and the effect of these processes on the H^- ion beam optics by using the 3D3V PIC simulation.

- The energy relaxation of H^- ions due to the Coulomb collision and the charge exchange is verified (T_{H-} = 1.5 eV → 0.49 eV).

- It is indicated that the Coulomb collision is dominant for the energy relaxation processes under the present calculation condition ($n_e = 1.0 \times 10^{18}$ m^{-3}, T_{H+} = 0.25 eV, n_H/n_{H2} =0.5, $n_H = 9.4 \times 10^{18}$ m^{-3}, T_H = 0.1 eV).

- It is shown from the emittance diagrams that the H^- ion beam optics is improved by the energy relaxation processes, and the separation of the beam core and the beam halo in the emittance diagram becomes clearer.

Future Plane

The 3D3V PIC model will be extended to include the accelerator. The simulation results of the accelerated H^- ion beam emittance and the heat loads in the accelerator will be compared with the experimental results.