Numerical analysis of isotope effect in NIFS negative ion source

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Summary

- In hydrogen (H) and deuterium (D) experiments in NIFS-RNIS, increase in co-extracted electron current is observed.
- For analysis of isotope effects in the ion source through electron transport simulation, 3D kinetic particle tracking model KEIO-MARC code was modified for application to NIFS-RNIS.

- KEIO-MARC code reproduced basic characteristics, such as electron flow by magnetic drift, filter effect, etc. and calculated EEDF, electron density, electron temperature, and reaction frequency.
- The isotope effects via following process was analyzed and we concluded that other isotope effects are the reason of difference in electron density.
  1. **Sheath potential drop** at the chamber wall did not produce large difference in electron density.
  2. **Coulomb collision** did not produce large difference in electron density.
  3. **Some reactions** between ground state atoms and molecules did not produce large difference in electron density.

1. Introduction

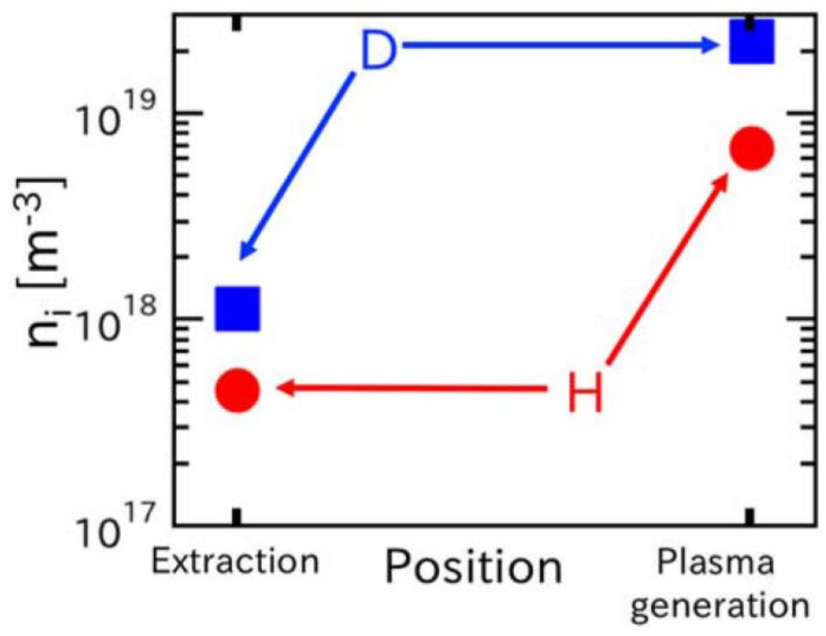

Fig. 1 Result of NIFS-RNIS experiment [1]

- In hydrogen (H) and deuterium (D) experiments in NIFS-RNIS (negative ion source for experiment), the electron density in both extraction and plasma generation region is higher in the D plasma than that of H plasma by a factor of around 3.[1]
- This will lead to NBI (Neutral Beam Injection) beam power limitation due to larger heat load by co-extracted electron current and needs to be improved.

Purpose

Investigation of high electron density in D plasma through electron transport simulation.

In this paper

Analysis of the isotope effect on 1. sheath potential drop, 2. coulomb collision, and 3. some reactions.

2. Simulation Model

KEIO-MARC code[2,3]

Kinetic modeling of **E**lectrons in the **IO**n source plasmas by the **M**ulti-cusp **ARC**-discharge code

KEIO-MARC code is a 3D kinetic particle tracking model which simulates electron transport through equation of motion.

$$m_e \frac{d\boldsymbol{v}_e}{dt} = -e\boldsymbol{v}_e \times \boldsymbol{B} + (\text{collision force})$$

※$E = 0$ by assuming quasi-neutral plasma in the chamber.

Considers…
- 3D shape of the target device.
- 3D magnetic configuration.
- Reflection at the chamber wall by sheath potential.
- Coulomb collisions.
  - 2 types of collisions: electron – electron collision and electron - H^+ collision.
  - H^+ density will be same as electron density by assuming quasi-neutral plasma because H^+ is treated as background plasma in this model.
- Both elastic and inelastic collisions.
  - $H_2, H^0, H^+, H_2^+, H_3^+$ are treated as background plasma. Density and temperature are given as a set parameter and spatial distribution is set to be uniform in the chamber.
  - When electron production reactions occurs, it produces 1 test particle (electron) at the reaction position and produced particle will be tracked as well.
  - When electron reduction reactions occurs, that test particle is lost at the reaction position.

Electron Energy Distribution Function (EEDF) is calculated for each spatial cell

NIFS-RNIS

Target device is R&D negative ion source NIFS-RNIS.

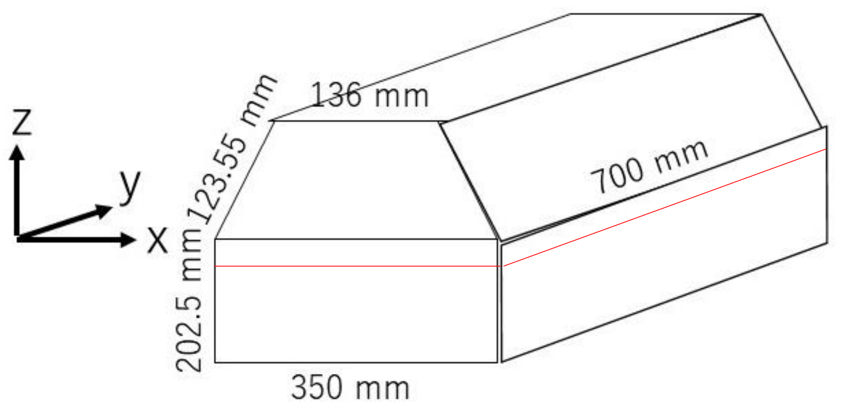

Fig. 2 Arc chamber dimension of NIFS-RNIS

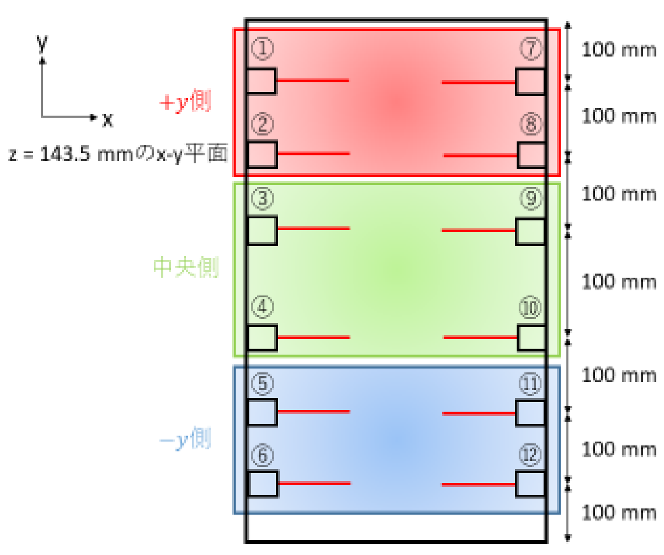

Fig. 3 Filament position

- $+Z$ axis direction : Opposite of beam extraction direction
- $+X$ axis direction : Parallel to filter magnetic field

Calculation Conditions

- Time step width : 10^{-10} [s]
- Time step number : 900,000
- Extraction holes : $z = 0$
- Weight of test particle : 3.13×10^{13}

Table 1 Arc-discharge conditions

Arc Power	8300 W
Arc Voltage	82 V
H_2 Gas Pressure	0.3 Pa

Table 2 Background plasma

Particles	Density [m^{-3}]	Temperature [K]
H_2	1.68×10^{18}	774
H^0	1.68×10^{17}	774
H^+	4×10^{17}	457
H_2^+	1×10^{17}	457
H_3^+	5×10^{17}	457

Reference

[1] H. Nakano, *et al.*, Jpn. J. Appl. Phys, 59 SHHC09 (2020).
[2] T. Shibata, *et al.*, J, Appl, Phys, 114 143301 (2013).
[3] A. Hatayama, *et al.*, New J. Phys., 20 065001 (2018).
[4] T. Shibata, *et al.*, 68 in this conference

3. Results and Discussion

Application to NIFS-RNIS

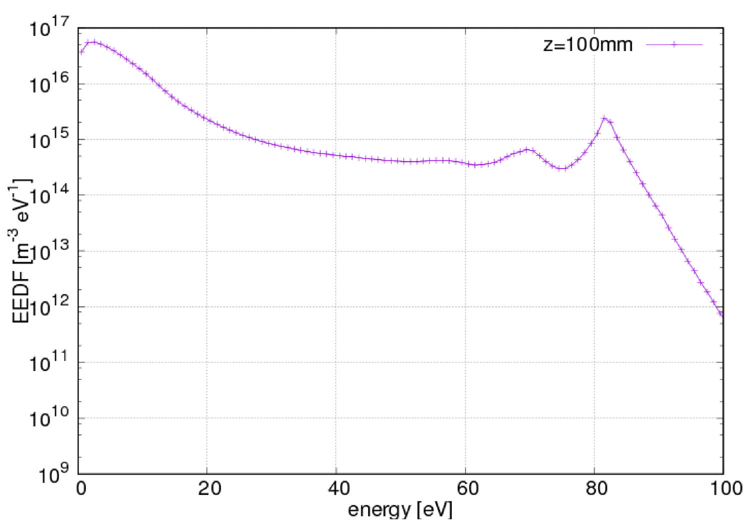

Fig. 4 EEDF

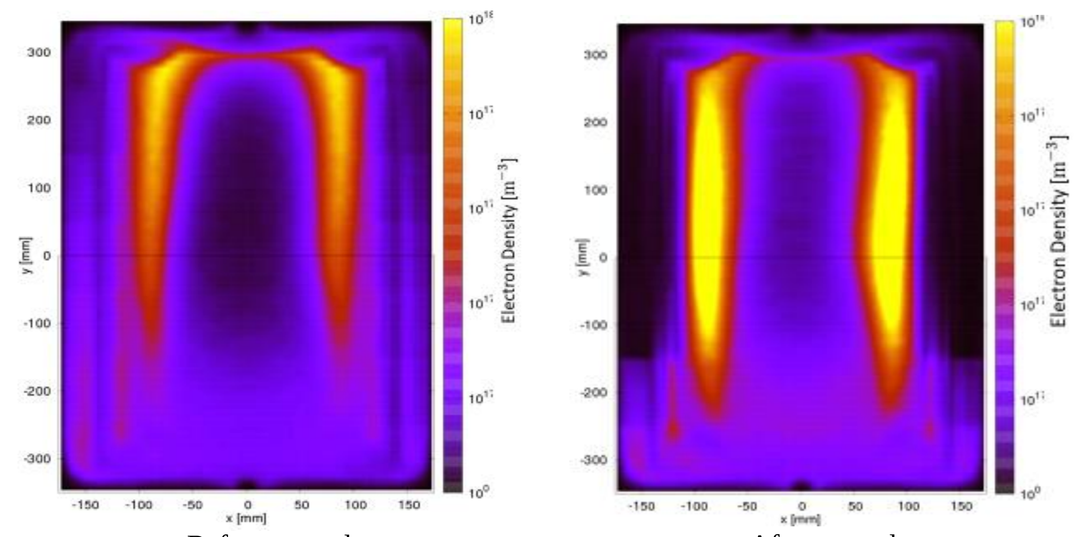
Before control
After control
Fig. 5 n_e distributions in xy plane at z = 142 mm (near filament)

Table 3 Production Reactions

Nondissociative Ionization	$e + H_2(X^1\Sigma_g^+) \rightarrow H_2^+ + 2e$
H(1s) Ionization	$e + H(1s) \rightarrow H^+ + 2e$
H_2^+ Dissociation 1	$e + H_2^+ \rightarrow H^+ + H^+ + 2e$
Dissociative Ionization	$e + H_2(X^1\Sigma_g^+; v = 0) \rightarrow H^+ + H(1s) + 2e$

Table 4 Reduction Reactions

Dissociative Attachment	$e + H_2(v) \rightarrow H + H^-$
H_2^+ Dissociation 3	$e + H_2^+ \rightarrow H(1s) + H^*$
H_3^+ Dissociative Recombination	$e + H_3^+ \rightarrow 3H(1s)$

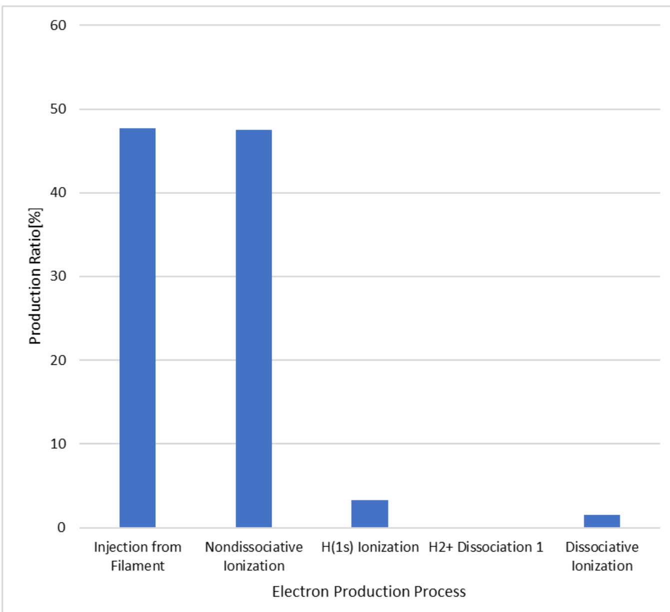

Fig. 6 Ratio of electron production process

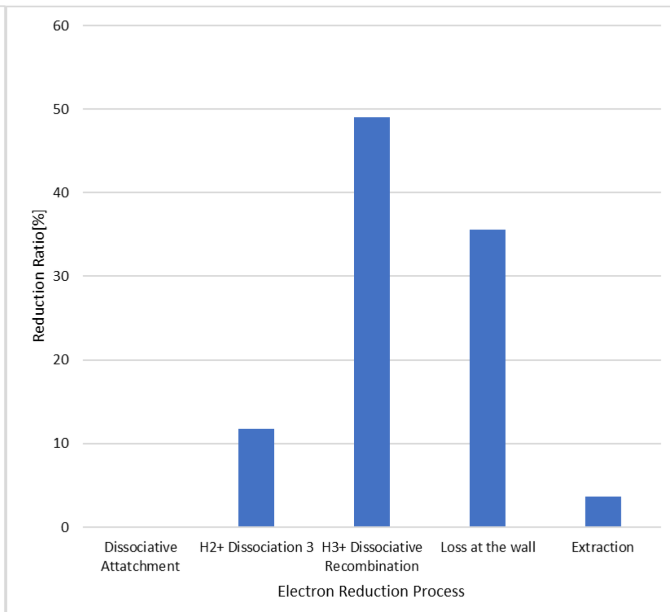

Fig. 7 Ratio of electron reduction process

- In EEDF, peak at 83 V (arc voltage) is observed.
- Filament injection control done in NIFS-RNIS to counter grad B drift is reproduced.
- Injection from filament and nondissociative ionization are the 2 dominant electron production process.
- H_3^+ dissociative recombination is the dominant electron reduction process, followed by loss at the wall.

1. Isotope effect on sheath potential drop

- Depth of sheath potential :

$$\Phi_{sh} = \frac{k_B T_e}{2e} \ln\left(\frac{m_i}{2\pi m_e}\right)$$

Table 5 Isotope effect on sheath potential drop

Electron Density Ratio	Electron Temperature Ratio
104.41%	99.57%

- Isotope effect on sheath potential drop is not the reason of electron density increase.

2. Isotope effect on coulomb collision

- Mass of collision partner : $m_{H^+} \rightarrow m_{D^+}$

Table 6 Isotope effect on coulomb collision

Electron Density Ratio	Electron Temperature Ratio
100.05%	100.24%

- Isotope effect on coulomb collision is not the reason of electron density increase.

3. Isotope effect on reactions

- Cross section
- Mass of collision partner

Table 7 Isotope effect on reactions

Reaction		Electron Density Ratio	Electron Temperature Ratio
DI	$e + H_2(X^1\Sigma_g^+; v = 0) \rightarrow e + H^+ + H(1s)$	99.81%	100.09%
Nondiss IOZ	$e + H_2(X^1\Sigma_g^+) \rightarrow e + H_2^+ + e$	99.40%	100.94%
DA	$e + H_2(v) \rightarrow H + H^-$	99.96%	100.02%
eV①	$e + H_2(X^1\Sigma_g^+; v = 0) \rightarrow e + H_2(X^1\Sigma_g^+; v = 1)$	97.38%	97.66%
eV②	$e + H_2(X^1\Sigma_g^+; v = 0) \rightarrow e + H_2(X^1\Sigma_g^+; v = 2)$	100.25%	99.01%
e Excitation	$e + H_2(X^1\Sigma_g^+) \rightarrow e + H_2^*(B^1\Sigma_u^+)$	105.07%	100.51%

- Isotope effect on these 7 reactions are not the reason of electron density increase.

4. Development Plans and Discussion

Following factors need to be considered…

- Difference of energy loss through each reactions.
- Difference of threshold energy.
- Isotope effect of other reactions.
- Reactions of vibrationally excited molecules.
- Difference of vibrationally excited levels of molecules.
- Ambipolar diffusion

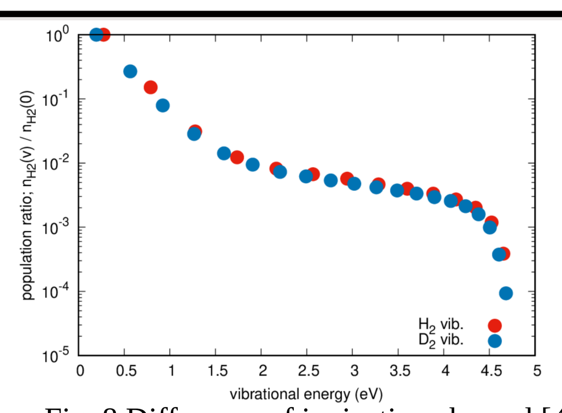

Fig. 8 Difference of ionization channel [4]

Calculation of the zero-dimensional model suggests that difference of vibrationally excited levels of molecules (H: 0~14, D: 0~20) is crucial because the difference of the ionization channel number via vibrationally excited levels is "one of the reasons for" the different ionization rate coefficients.[4]