Numerical study of different electron density observed in Hydrogen and Deuterium ion source plasmas

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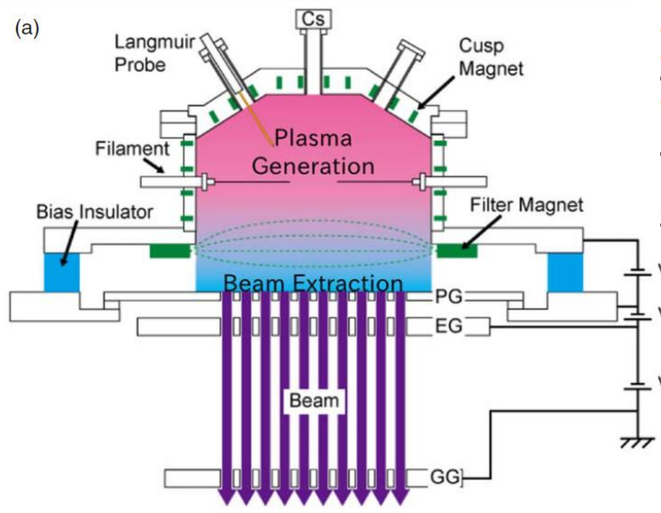
Abstract

Sequences of hydrogen (H) and deuterium (D) experiments have been done by NIFS research and development negative ion source (RNIS) for the deuterium NBI development. In the experiments, the co-extracted electron current with the negative ions and the electron density in the plasma generation region in the D experiment have been around three times higher than that in the H experiment. To explain the difference of the electron density in the RNIS driver region, a zero-dimensional numerical model is developed in the present study. The model only focuses on the isotope effect for vibrationally excited level of electronically grounded state molecules and its relevant cross-sections. The calculation results show that difference of the ionization channel numbers via molecular vibrationally excited states could be a reason to enhance ionization rate in D plasma.

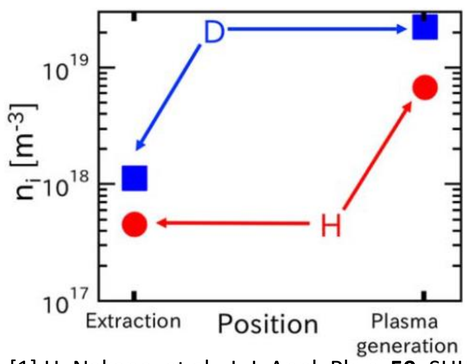
NIFS LHD-NBI and RNIS experiments



Operation parameters of RNIS	
Arc current	600 A (P_{arc} = 50 kW)
Gas flow rate	850 sccm (for H2 exp.)

Table I. Comparison of extracted current characteristics between hydrogen and deuterium operations. The I_e, $I(H^-)$ and $I(D^-)$ are currents of co-extracted electron, H^- beam, and D^- ion beam, respectively. Other operation parameters except discharge power were the same in both operations.

Gas species	Discharge power [kW]	I_e [A]	$I(H^-)$, $I(D^-)$ [A]	$I_e/I(H^-)$, $I_e/I(D^-)$
H_2	165	9.3	24.6	0.38
D_2	149	22.6	16.5	1.37



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- In hydrogen (H) and **deuterium (D) Experiments in NIFS-LHD** operations, ratio of **the co-extracted electron current** to the negative ion current is **higher** in the D experiments **by a factor of around 3**.
- In NIFS RNIS (R&D Negative Ion Source) experiment, **the electron density** in the extraction region and in the plasma generation region is also **higher in the D plasma** than in that of the H plasma **by a factor of 3.**
- **For the investigation** of the high electron density in D plasma, we developed **a zero-dimensional model** which focuses on the **isotope effect for the vibrationally excited levels of H_2 and D_2 molecules**.

Isotope Effects for vibrationally excited levels of H_2 and D_2

- **Mass Scaling of vibrationally excited molecular levels** :

$$v' = \frac{\omega_{D2}}{\omega_{H2}} \times v_i = \sqrt{\frac{\mu_{H2}}{\mu_{D2}}} \times v_i$$

- **Franck-Condon Factor**: $F_{v_i,v_f}^{N^1,X^1} = \left|\int_0^\infty \varphi_{v_i}^{*\,N^1}(r)\, \varphi_{v_f}^{X^1}(r) dr\right|^2$
- **Einstein Coefficient (for spontaneous radiation and EV process):**

$$A_{v_i,v_f}^{N^1,X^1} = \frac{16}{3}\frac{\pi^3}{\varepsilon_0 h}\frac{1}{\lambda^3}\left|\int_0^\infty \varphi_{v_i}^{*\,N^1}(r)\, D_{el}(r) \varphi_{v_f}^{X^1}(r) dr\right|^2$$

#	Reactions
1	$H_2(X^1\Sigma_g^+; v_i) + e^- \rightarrow H_2(N^{1,3}\Lambda_\sigma) + e^- \rightarrow 2H + e^-$
2	$H_2(X^1\Sigma_g^+; v_i) + e^- \rightarrow H_2(B^1\Sigma_u^+ \text{ or } C^1\Pi_u) + e^- \rightarrow H_2(X^1\Sigma_g^+; v_f) + e^- + h\nu$
3	$H_2(X^1\Sigma_g^+; v_i) + e^- \rightarrow H_2(X^1\Sigma_g^+; v_f = v_i \pm 1) + e^-$
4	$H_2(X^1\Sigma_g^+; v_i) + e^- \rightarrow H_2^+(X^2\Sigma_g^+) + 2e^-$
5	$H_2(X^1\Sigma_g^+; v_i) + e^- \rightarrow H_2^+(X^2\Sigma_g^+) + 2e^- \rightarrow H + H^+ + 2e^-$
6	$H_2(X^1\Sigma_g^+; v_i) + e^- \rightarrow H_2^-(X^2\Sigma_u^+) \rightarrow H^- + H$
7	$H_2^+(X^2\Sigma_g^+) + e^- \rightarrow H_2^+(2p\sigma_u,^2\Sigma_u^+) + e^- \rightarrow H + H^+ + e^-$
8	$H_2^+(X^2\Sigma_g^+) + e^- \rightarrow H_2^{*Ryd}(N^{1,3}\Lambda_\sigma) \rightarrow 2H$
9	$H_2^+(X^2\Sigma_g^+) + e^- \rightarrow 2H^+ + 2e^-$
10	$H_3^+ + e^- \rightarrow H_3^+(N^{1,3}\Lambda_\sigma) + e^- \rightarrow H^+ + H_2(X^1\Sigma_g^+; v_f) + e^-$
11	$H_3^+ + e^- \rightarrow H_3^{*Ryd}(N^{1,3}\Lambda_\sigma) \rightarrow 3H \text{ or } H_2(X^1\Sigma_g^+; v_f) + H$
12	$H_2(X^1\Sigma_g^+; v_i) + H_2^+ \rightarrow H_3^+ + H$
13	$H + e^- \rightarrow H^+ + 2e^-$
14	$H^+ + e^- \rightarrow H + h\nu$

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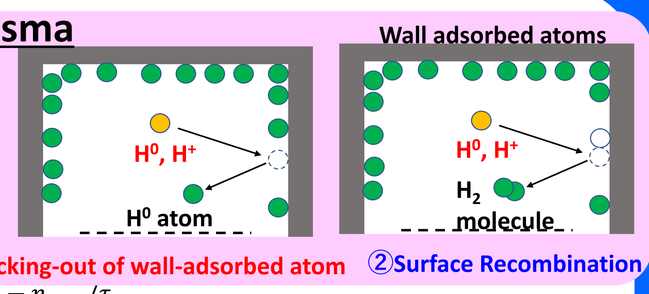
A zero-dimensional model for H_2 and D_2 plasma



RATE EQUATIONS

Electron:

$$\frac{dn_e}{dt} = S_{IOZ-H} + S_{IOZ-H2} - S_{RCMB} + S_{DI} + S_{filament} - n_e/\tau_e$$

Positive ions:

$$\frac{dn_{H+}}{dt} = S_{DI} - S_{RCMB} + S_{IOZ-H} + S_{DE-H2+} - n_{H+}/\tau_+$$
$$\frac{dn_{H2+}}{dt} = S_{IOZ-H2} - S_{DR} - S_{DE} - S_{DI-H2+} + S_{DE-H3+} - S_{H3+PROD} - n_{H2+}/\tau_+$$
$$\frac{dn_{H3+}}{dt} = -S_{DR} - S_{DE-H3+} + S_{H3+PROD} - n_{H3+}/\tau_+$$

①Kicking-out of wall-adsorbed atom

Atom: $\frac{dn_H}{dt} = \sum_v S_{DISS-H2}(v) + S_{RCMB-H+} - S_{IOZ-H} + S_{DISS} + S_{DI} + S_{DE} + S_{DR} - \frac{n_H}{\tau_H} + \boldsymbol{R_{N+} \times \frac{n_{H+}}{\tau_+} + R_{N0} \times \frac{n_{H0}}{\tau_{H0}}}$

②Surface Recombination

Mol.: $\frac{dn_{H2}(v)}{dt} = -S_{DISS}(v) - S_{IOZ-H2}(v) - \sum_{v_f} S_{EVB,C}(v, v_f) + \sum_{v_i} S_{EVB,C}(v_i, v)$
$+S_{eV}(v \pm 1) - S_{eV}(v) + S_{gas}(v = 0) - n_{H2}/\tau_{H2} + \boldsymbol{0.5 \times (1 - R_{N+}) \times \frac{n_{H+}}{\tau_+} + 0.5 \times (1 - R_{N0}) \times \frac{n_{H0}}{\tau_{H0}}}$

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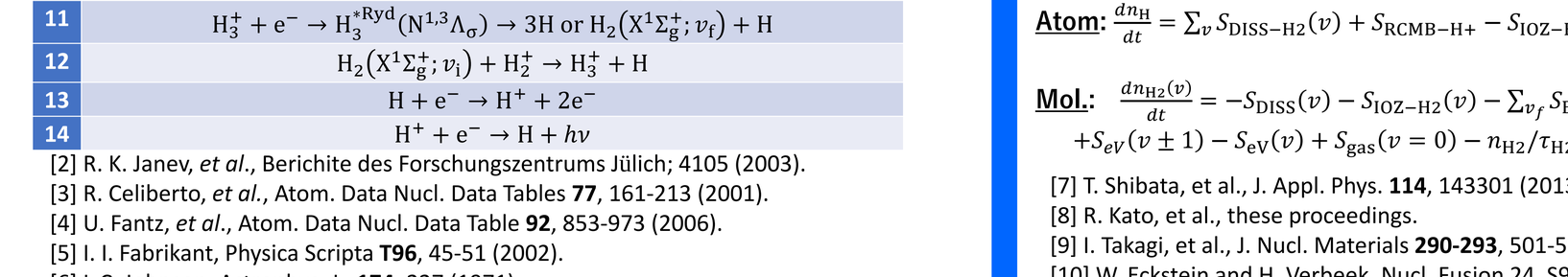
Temperature (fixed)	
Electron	5.0 eV
Positive Ions	1.0 eV
Neutrals	0.1 eV (~1000 K)

Characteristic time for transport loss	
Electron & positive ions	$\tau_e = \tau_+ = 1 \times 10^{-5}$s
H2/D2 molecules	$\tau_{H2} = 5 \times 10^{-3}$s
H/D atoms	$\tau_H = 1 \times 10^{-3}$s

Wall Reflection Probability as Atoms	
For Incoming H^+/D^+	R_{N+} = 90.95 %
For Incoming H/D	R_{N0} = 95.55 %

- **The isotope effects** taken into account in this model is **only "difference of vibrationally excited levels of H_2 and D_2 molecules"** and the relevant reaction cross-section (with the Franck-Condon factor and the A coefficient for spontaneous radiation).
- **A zero-dimensional (0D) model** solves rate equations for **molecules** (each vibrationally excited levels in electronically grounded state), **atoms, positive ions (H^+, H_2^+, H_3^+ or D^+, D_2^+ D_3^+) and electrons.**
- The reactions (in the table) for the H plasma and the D plasma are applied to the 0D model individually to obtain the steady-state electron density.
- **The reaction rates** for electron impact processes are calculated from EEDF which is assumed to by Maxwellian distribution with T_e = 5.0 eV.
- **Characteristic transport loss time** for each particle species are fixed and given in the rate equations in the form of "$-n/\tau$".
- **The H atoms and H+ ions** (or D atoms and D+ ions) **incoming to the wall are reflected** as atoms or molecules. We assume that the wall is fully covered by H atoms. Most part of the reflection is **"kicking out of wall absorbed atoms"** with probability over 90%. The other part is **"surface recombination"** given in the probability $(1 - R_{N+})$ and $(1 - R_{N0})$, which is below 10%.

The H_2/D_2 Isotope Effects appear in the steady-state electron density difference



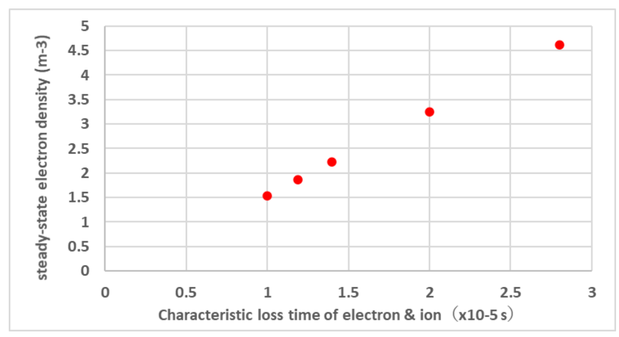
Steady-state density(m^{-3})	H_2 model	D_2 model
e^-	1.54E+19	2.54E+19
H^+	1.48E+19	2.48E+19
H^0	1.06E+20	1.08E+20
H_2 (v=0)	2.76E+17	2.36E+17
H_2^+	2.06E+15	2.13E+15
H_3^+	2.14E+12	9.09E+11

Main Reaction Rate Coefficients ($m^3\ s^{-1}$) (Rate)/ne/nH2(v=0)	H_2 model	D_2 model
Non-Dissociative EXC $X^1 - B^1$	1.56E-15	2.02E-15
Dissociative EXC $X^1 - B^1$	3.53E-17	4.99E-17
Dissociative EXC $X^1 - C^1$	4.00E-17	5.67E-17
Dissociative EXC $X^1 - b^3$	1.51E-14	1.77E-14
Non-Dissociative Ionization from X^1	9.88E-16	1.17E-15
Dissociative Ionization from X^1	3.32E-18	4.19E-18

- **From the calculation, the higher electron (and D^+) density are obtained in the D_2 model**.
- The rate coefficient of ionization process (including all vibrationally excited levels) is higher in the D_2 model, however, dependence of the vibrationally excited levels to the vibrational energy matches in the H_2 and D_2 models.
- **The difference of the ionization channel number via vibrationally excited levels is the reason of the different ionization rate** coefficient in the H_2 and D_2 models. This isotope effect appear in the electron density difference.
- However, the ratio of the electron density in H_2 and D_2 models are around 1.65 while the ratio is around 3 in the experiments.
- We conclude that this difference due to the vibrationally excited levels is **one of the isotope effects.**

Other isotope effects (will be reported in the near future)

1. Characteristic transport loss time for electrons and positive ions



2. Electron Temperature