Towards Advanced Wall Modeling Using Machine Learning and Its Integration with Neutral Transport Simulations

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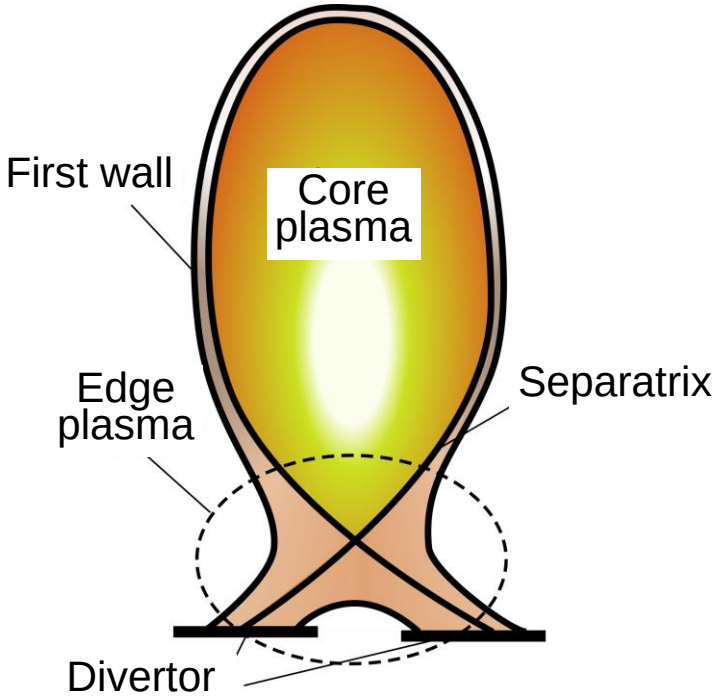
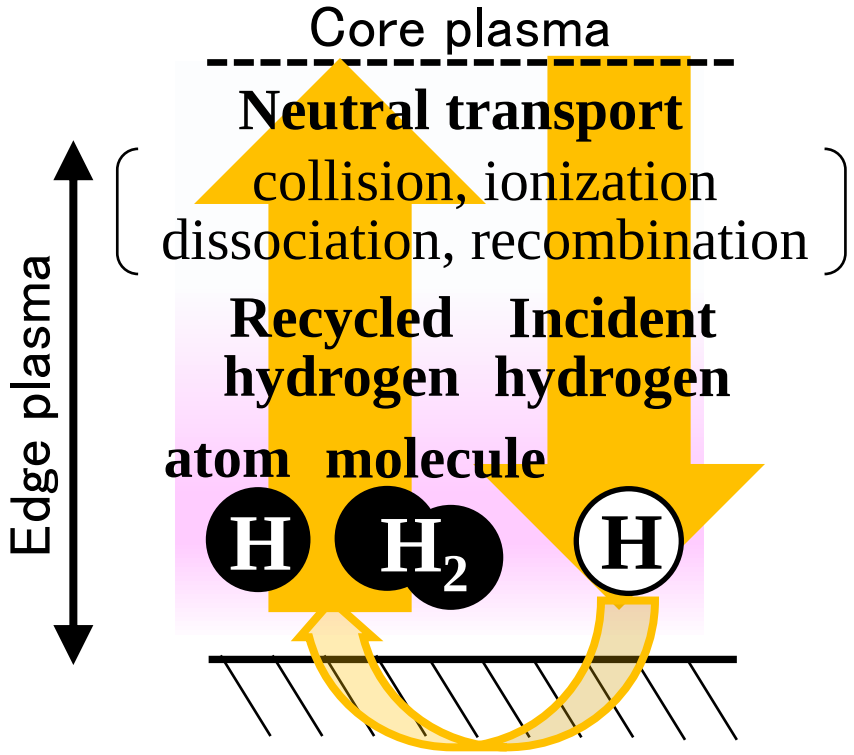
1. Background
2. Molecular dynamics simulation of hydrogen recycling on tungsten wall
3. Integration with fluid codes and neutral transport simulation
4. Machine learning approaches for the wall model
5. Future work: towards advanced wall modeling

Hydrogen recycling and plasma-material interaction





Hydrogen recycling on the wall

Changes in particle emission distribution

Plasma condition
- Density: n_e
- Elec. temp.: T_e
- Ion temp.: T_i

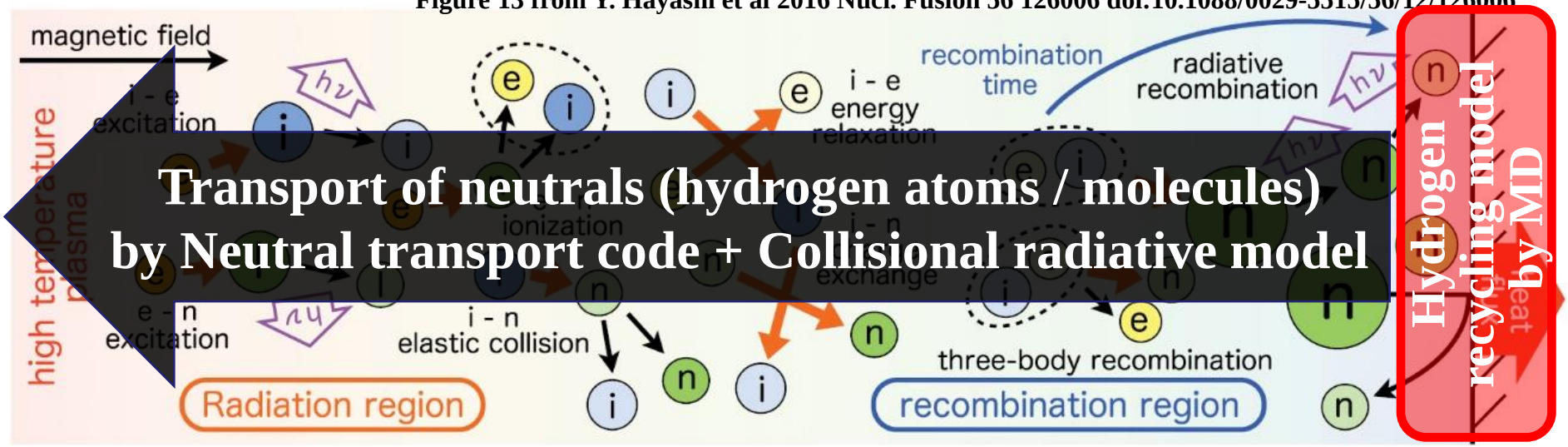
Interaction

Wall condition
- Mater. temp.: T_m
- Particle density: ρ
- Crystl. struct.

Changes in incident energy, flux, etc.

Background：Importance of detached plasma and hydrogen molecular processes

Figure 13 from Y. Hayashi et al 2016 Nucl. Fusion 56 126006 doi:10.1088/0029-5515/56/12/126006



Transport of neutrals (hydrogen atoms / molecules) by Neutral transport code + Collisional radiative model

Detached plasma

- Key technology to reduce heat load on the wall (prevent walls from melting)
- Neutral gas (hydrogen, nitrogen, neon, etc.) is injected into the divertor region to neutralize the plasma.

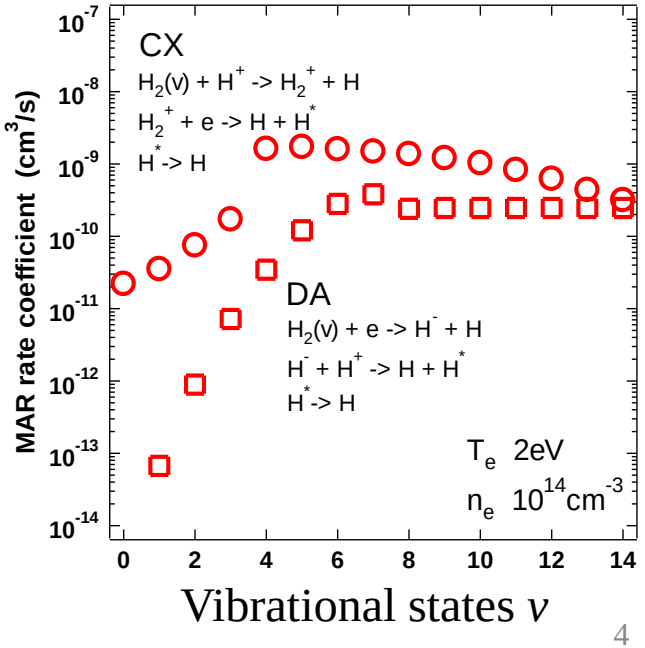
Molecular Assisted Recombination: MAR

Charge exchange recombination (CX) :

$$H_2 + H^+ \rightarrow H_2^+ + H, H_2^+ + e \rightarrow H + H^*, H^* \rightarrow H$$

Dissociative recombination (DA):

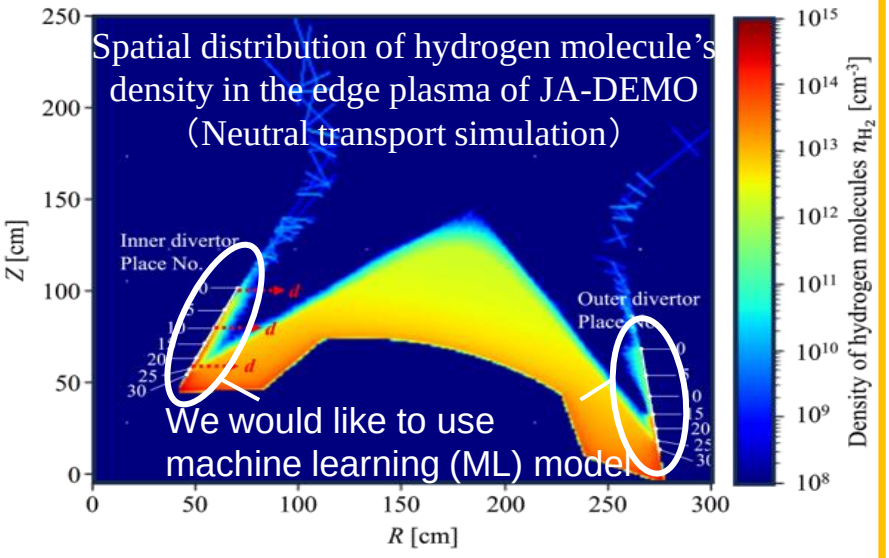
$$H_2 + e \rightarrow H^- + H, H^- + H^+ \rightarrow H + H^*, H^* \rightarrow H$$



Overview of our wall model

Context and Motivation

- We would like to calculate neutral transport in the edge plasma under the dynamically changing interaction between the plasma and the wall.
- By using machine learning, we can dynamically generate the distribution of released hydrogen (especially the rovibrational states of hydrogen molecules) from the plasma parameters near the wall.

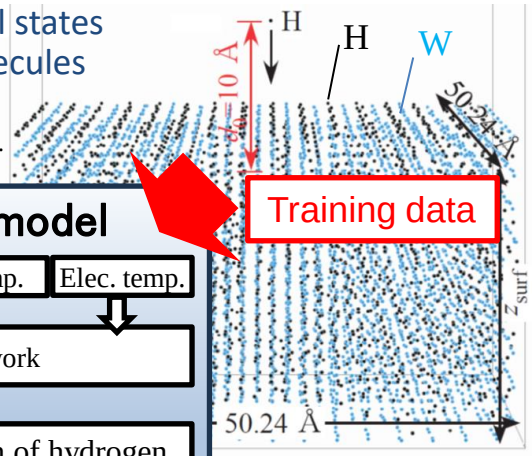


S. Saito, *et al*., Nucl. Fusion 64 126067 (2024).

① MD simulation

Evaluation of rovibrational states of emitted hydrogen molecules

- S. Saito, *et al*., Contrib. Plasma Phys. e201900152 (2020).
- S. Saito, *et al*., Jpn. J. Appl. Phys. 60, SAAB08 (2021).



Training data

② Training ML model

Input: H/W | Mater. temp. | Ion temp. | Elec. temp.

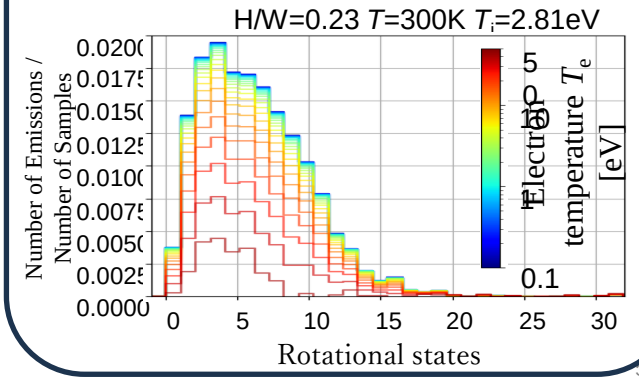
Fully connected network

Output: Output: emission distribution of hydrogen (translational energy, rovibrational states)

Prediction

③ Prediction of release distribution

Distribution of Rotational states of released hydrogen molecules



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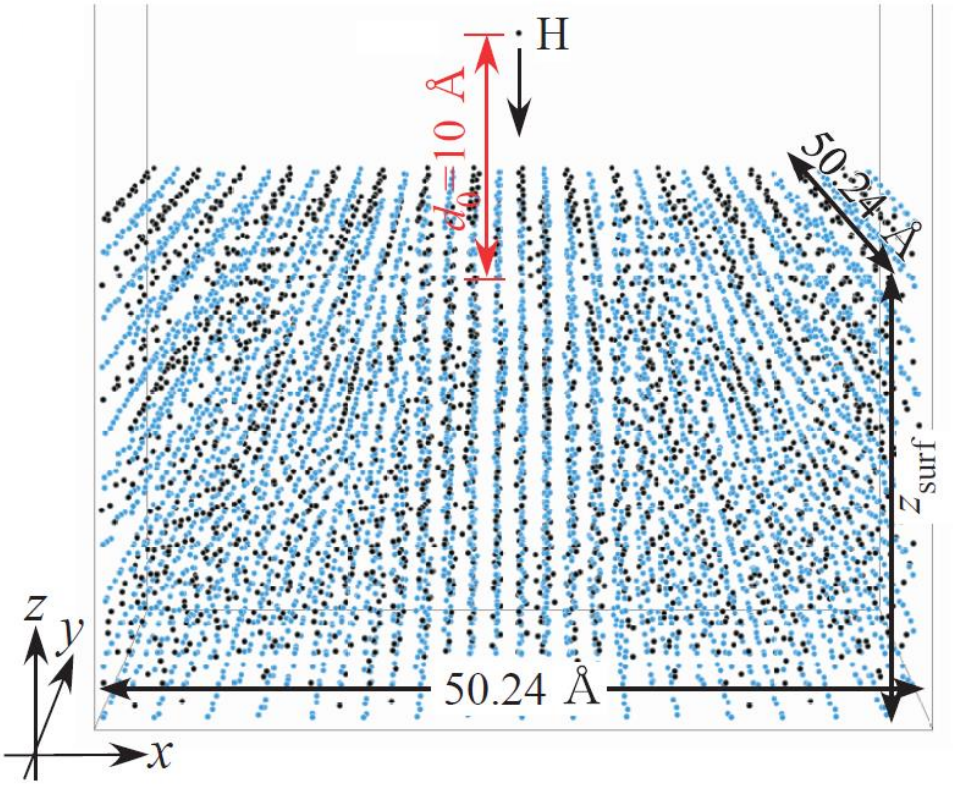
Hydrogen Recycling Model on Tungsten Materials（MD）



- Tungsten (W)
- Hydrogen (H)

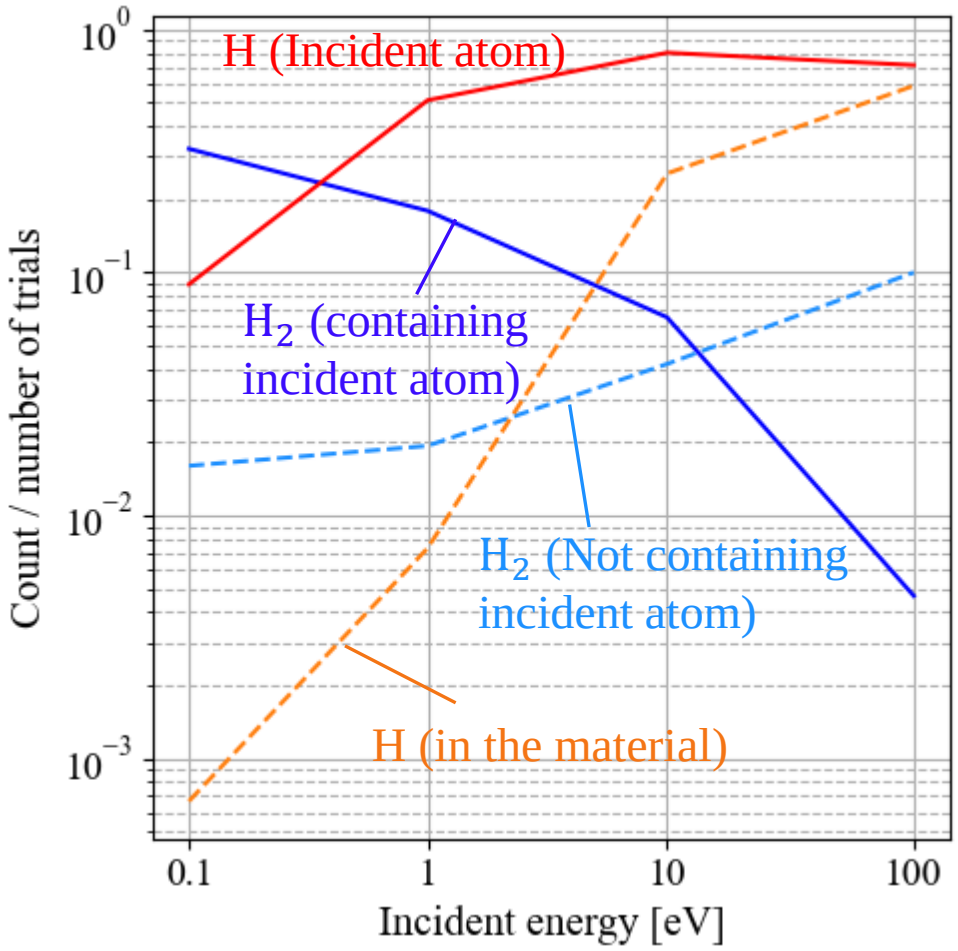
- Target material : Hydrogen contained bcc tungsten
- Boundary condition : Periodic in *x* and *y*
- Material temperature : 300 K
- Interaction : EAM potential [1]

- Incident atom : Hydrogen atom
- Number of Incidents : One
- Thermostat : Langevin
- Incident energy : 0.1-100 eV
- H/W : 0.2

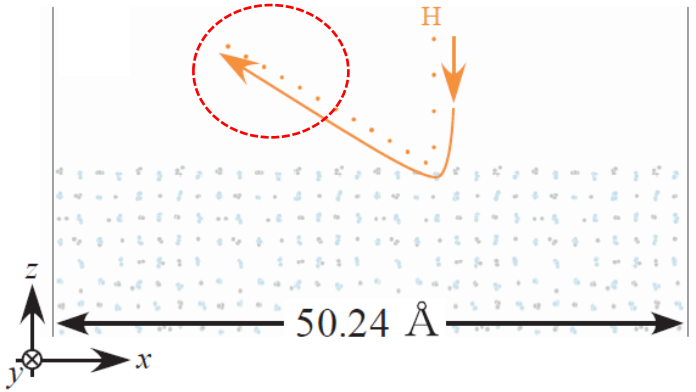
[1] Li-Fang Wang, Xiaolin Shu, Guang-Hong Lu, and Fei Gao: J. Phys. Condens. Matter **29** (2017) 435401.

Incident energy dependence of hydrogen emission

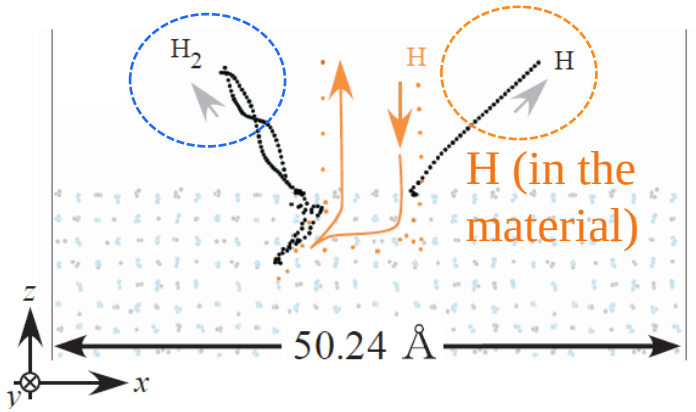
S. Saito, *et al.*, "*Emission of high rovibrational hydrogen molecules under detached plasma conditions by recycling on the tungsten wall*", Nuclear Fusion **64** 126067 (2024).



H (Incident atom)



H_2 (Not containing incident atom)

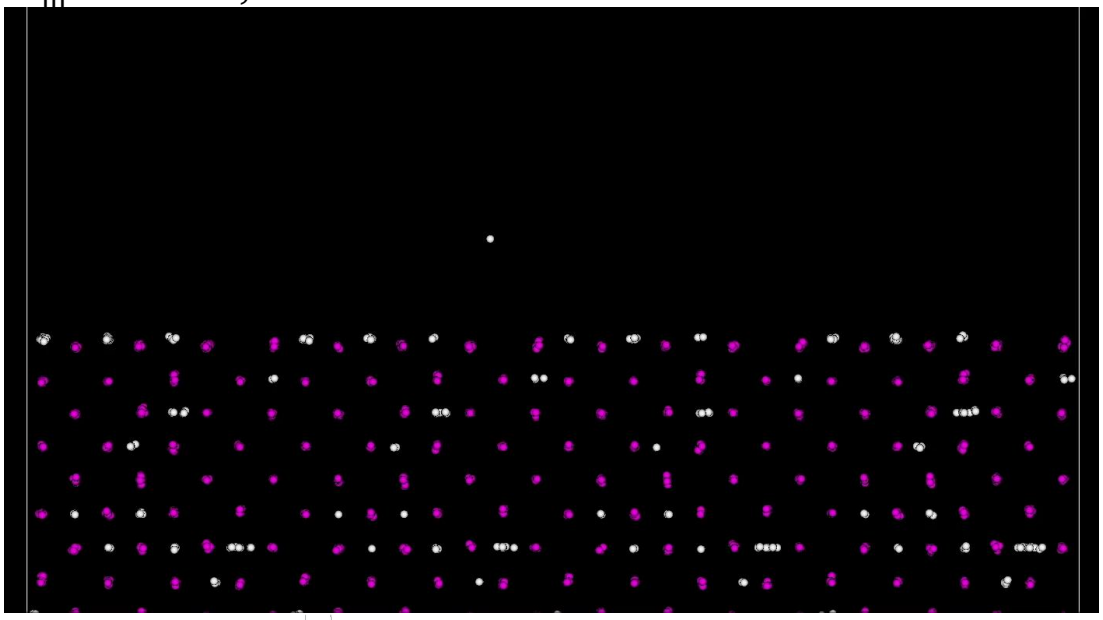


When the incident energy is low, many molecules containing incident hydrogen are emitted.
→ There is a possibility that a large amount of hydrogen molecules are released under detached condition.

Trajectory analysis of H_2 generation on the surface in low incident energy case

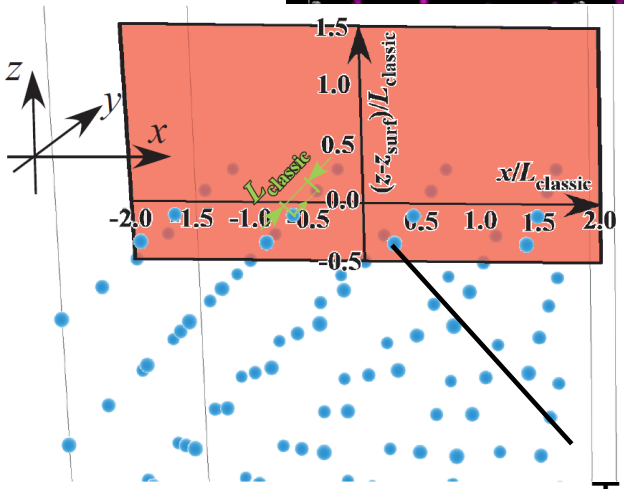
S. Saito et al., Jpn. J. Appl. Phys. **60**, SAAB08 (2021)

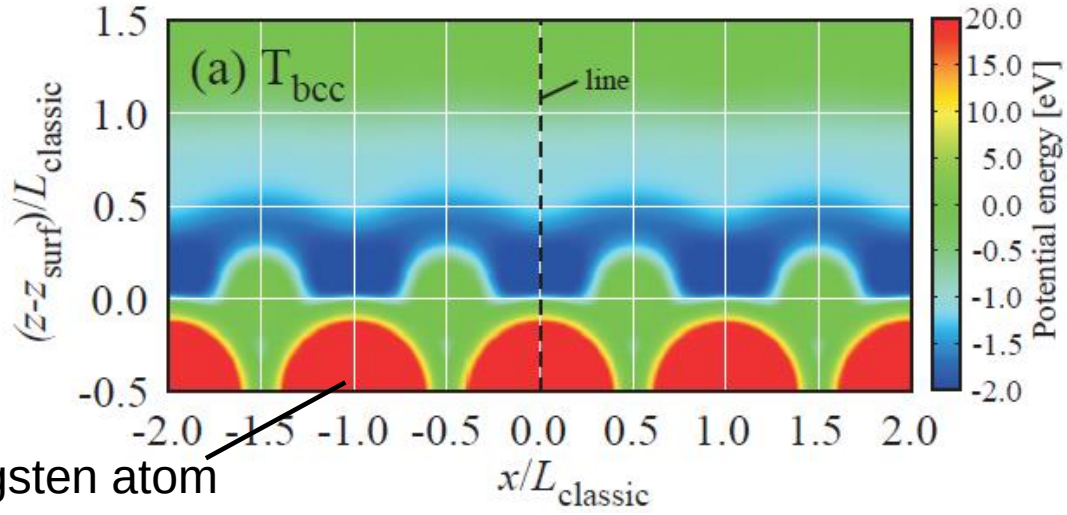
E_{in} = 0.1 eV, H/W=0.2



● Tungsten atom

○ Hydrogen atom



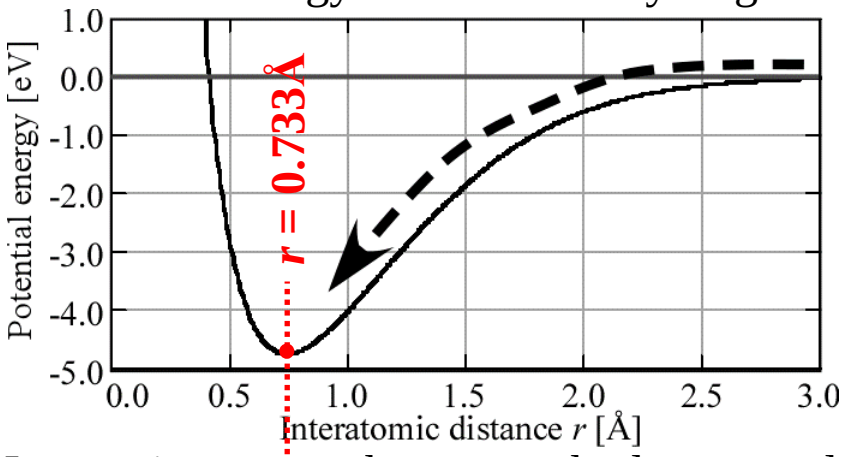


Tungsten atom

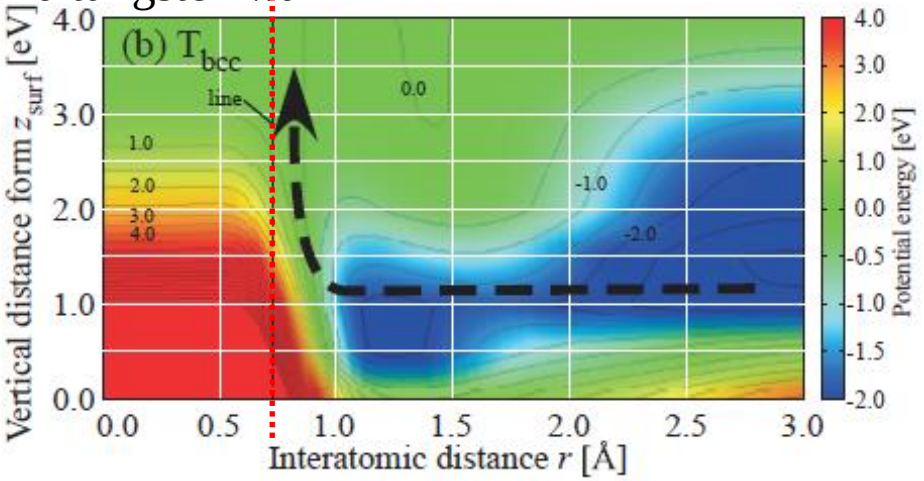
When the incident energy is low, most of the incident hydrogen atom forms molecules on the surface.

Energy acquisition mechanism of hydrogen molecules

Interaction energy between two hydrogen atoms

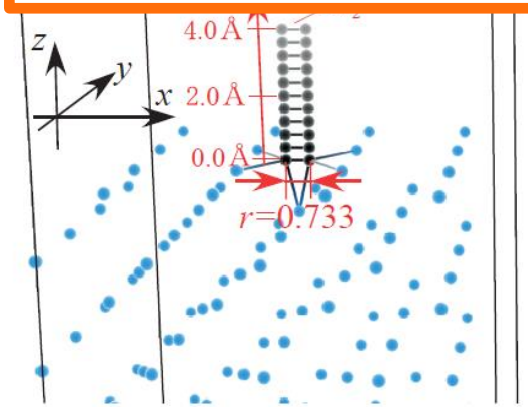


Interaction energy between a hydrogen molecule and tungsten wall

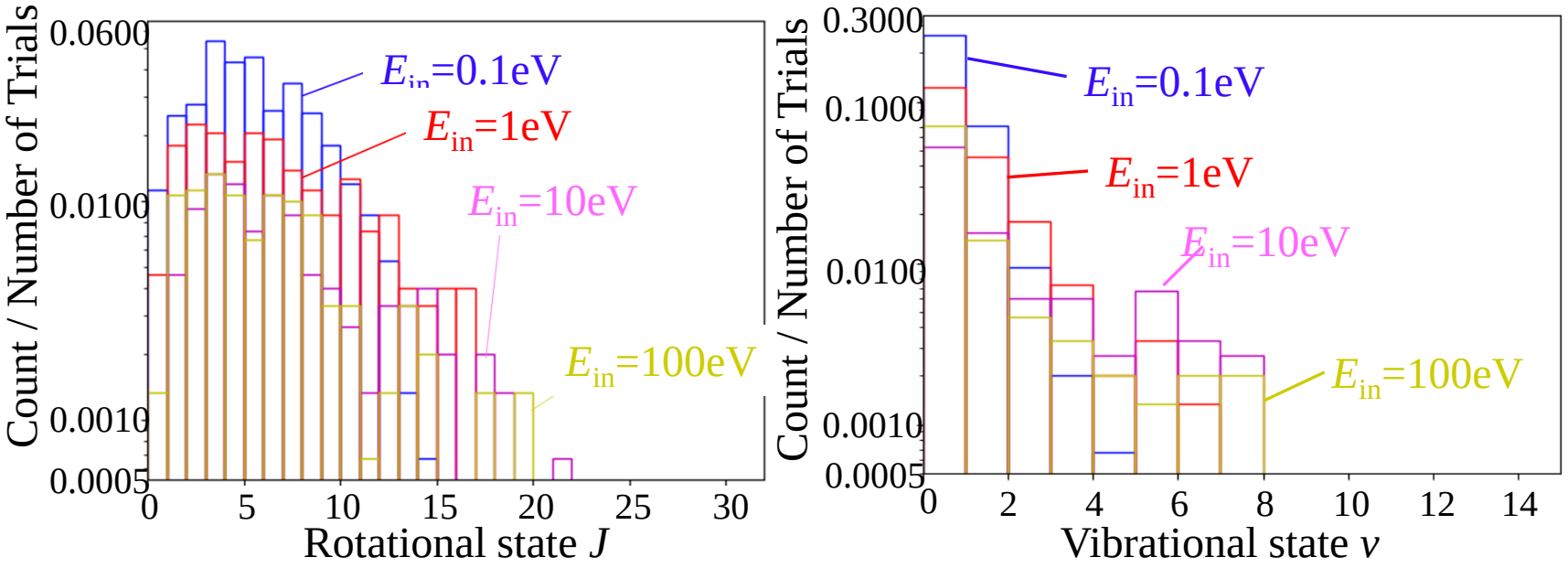


1. Incident hydrogen atoms acquire surface binding energy (~1.5 eV) when they are trapped on the surface.
2. When forming a molecule on the surface, the molecule acquires the binding energy (~4.5 eV) between two hydrogen atoms.
3. After forming a molecule on the surface, the molecule receive a repulsive force from tungsten wall and the molecule is accelerated (less than 1.0 eV?) in the vertical direction.

→ **Possibility of forming molecules with high rovibrational states**



Incident energy dependence of distribution of rovibrational states of released hydrogen molecules



Even if the incident energy is low, molecules with relatively high rovibrational states are formed.

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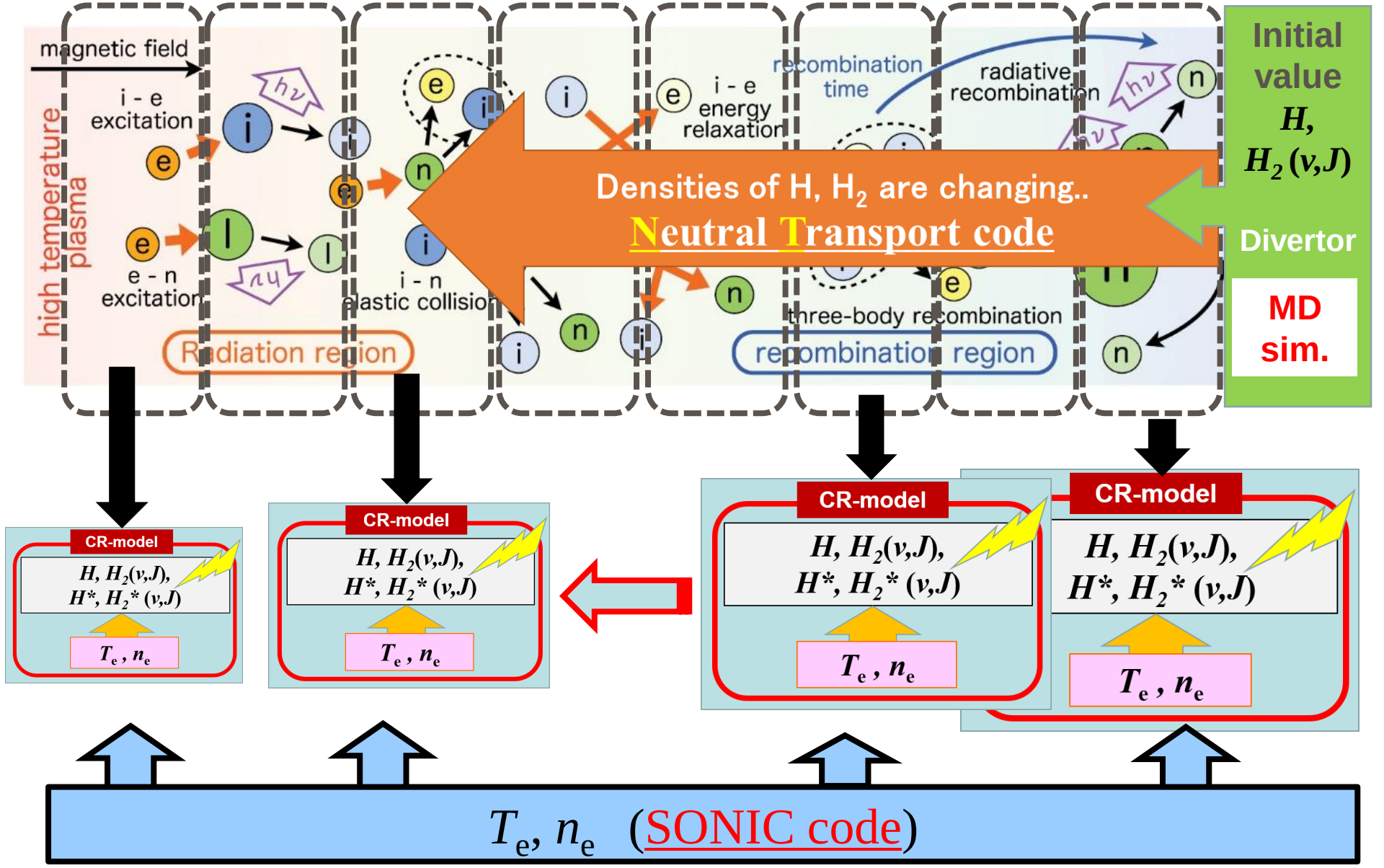
Combining NT-CR code, MD, and SONIC code

Figure 13 from Y. Hayashi, *et. al*. 2016 Nucl. Fusion 56 126006 doi:10.1088/0029-5515/56/12/126006

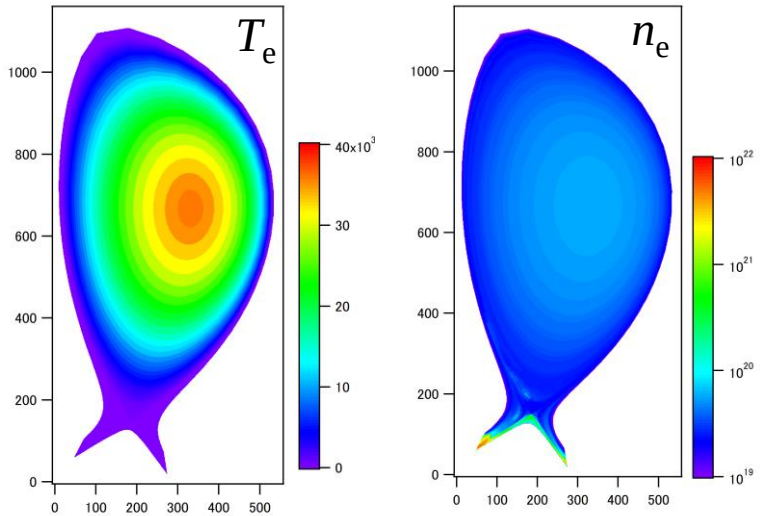


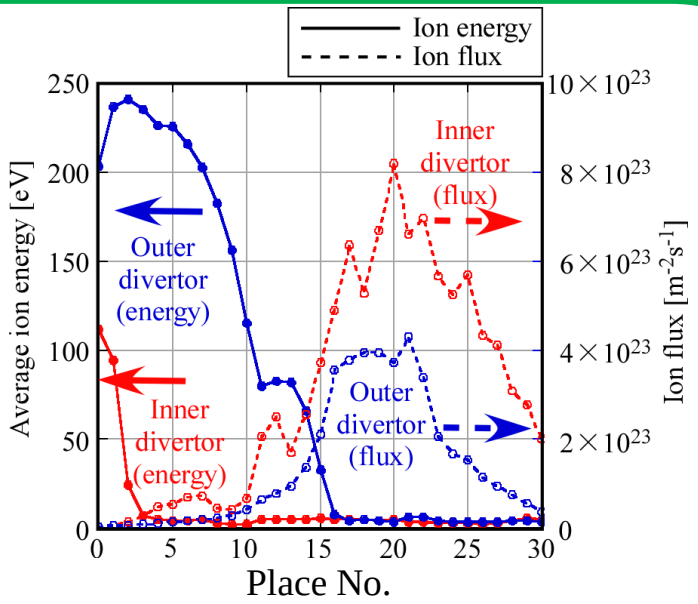
Neutral transport simulation with SONIC + MD for JA-DEMO

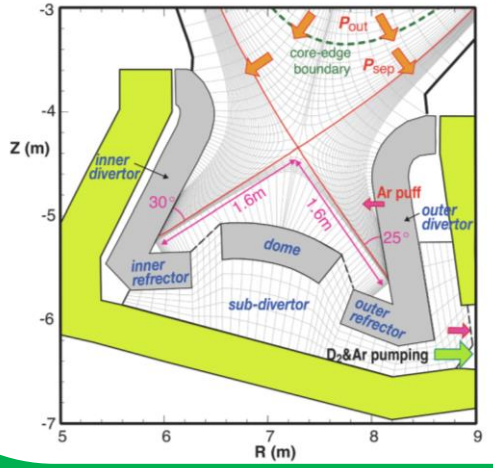
Emission distribution of rovibrational states (v, J) by MD sim.

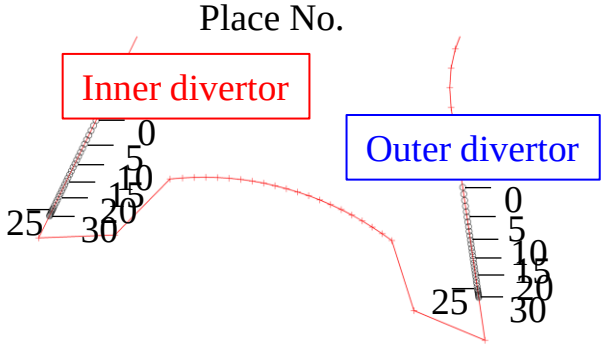
T_e & n_e by SONIC

NT simulation with CR model



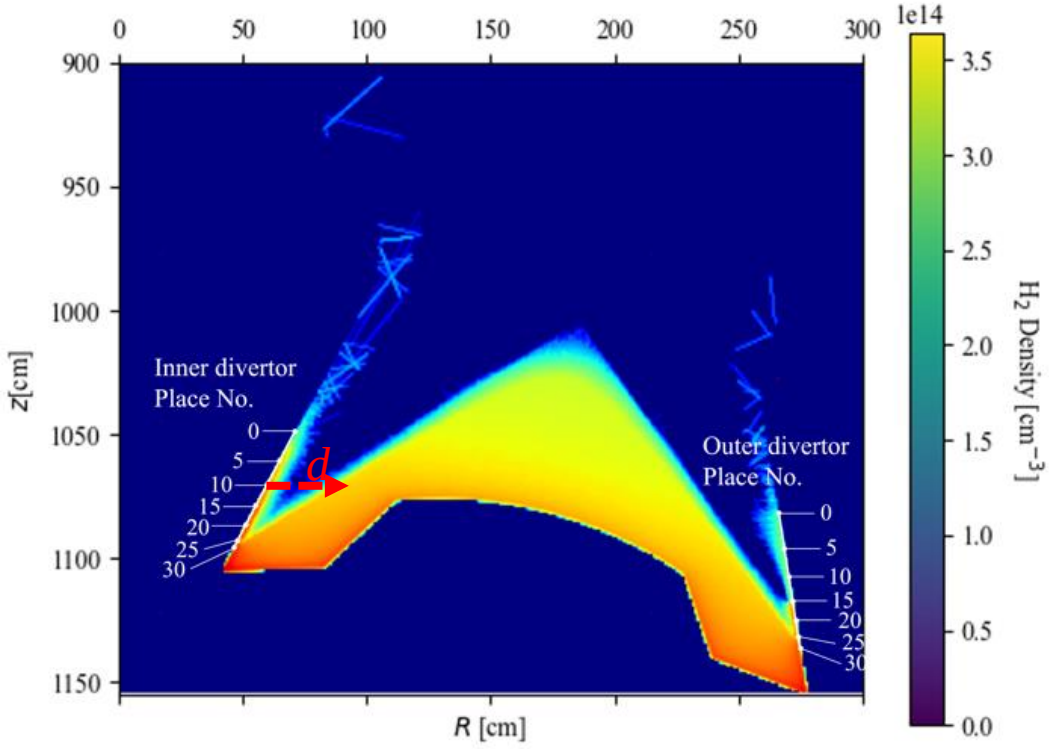


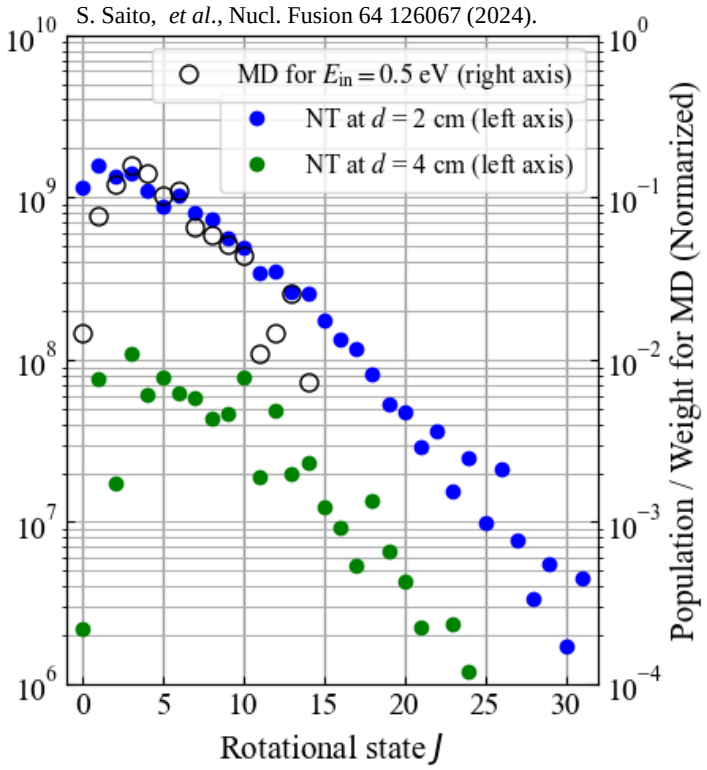




N. Asakura, K. Hoshino, Y. Homma, Y. Sakamoto, Joint Special Design Team for Fusion DEMO, “Simulation studies of divertor detachment and critical power exhaust parameters for Japanese DEMO design”, Nuclear Materials and Energy **26** (2021) 100864.

Spatial distribution of H_2 near divertor

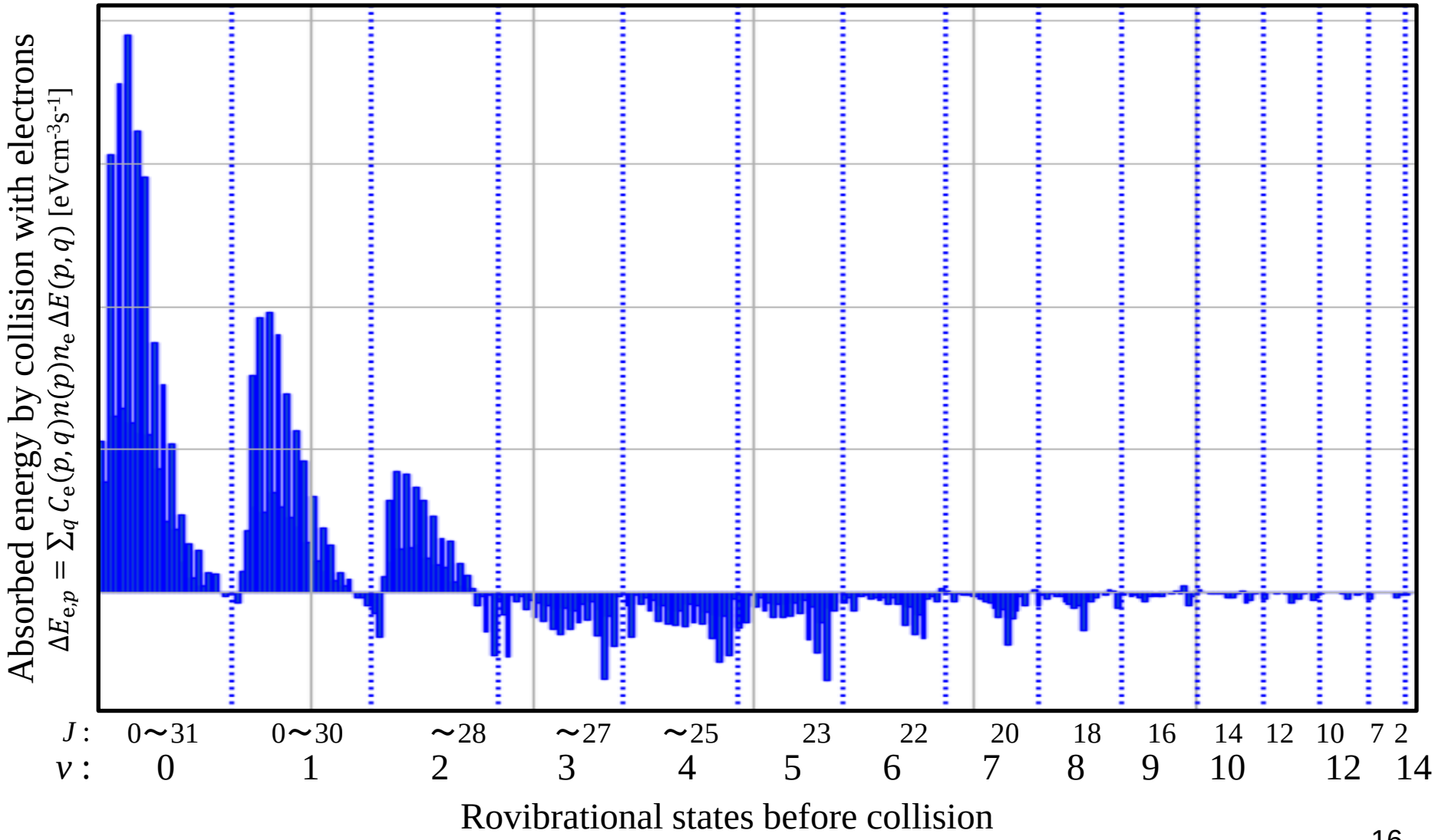




S. Saito, *et al.*, Nucl. Fusion 64 126067 (2024).

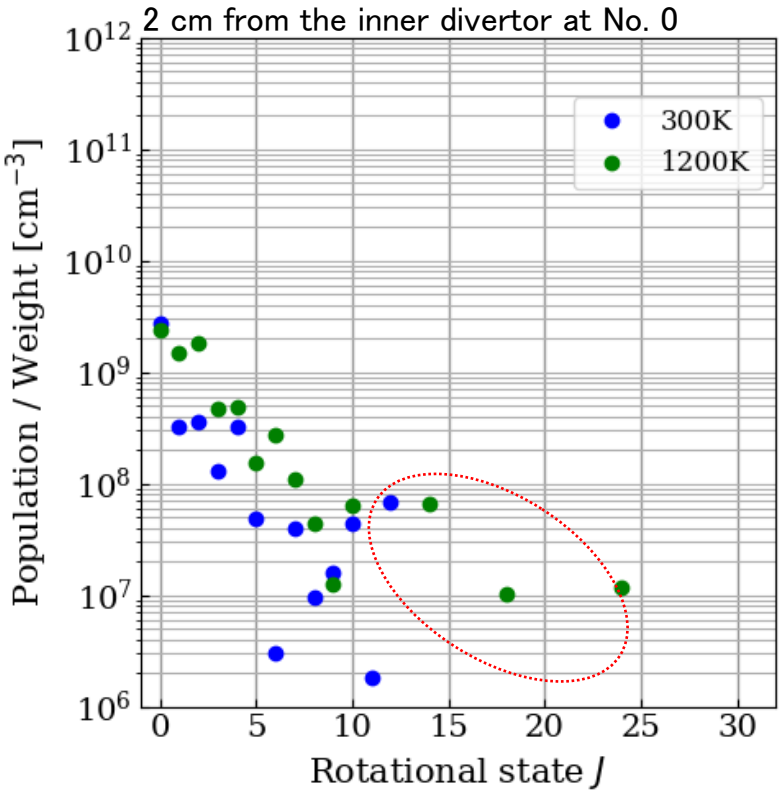
The data suggest that the molecules with rotational states higher than J=15 are produced by the collisions with electrons, H^+ ions, or neutral H atoms near the divertor, even though the absence of those higher-level molecules in the emission distribution.

Rovibrational state dependence of absorbed energy by collision with electrons

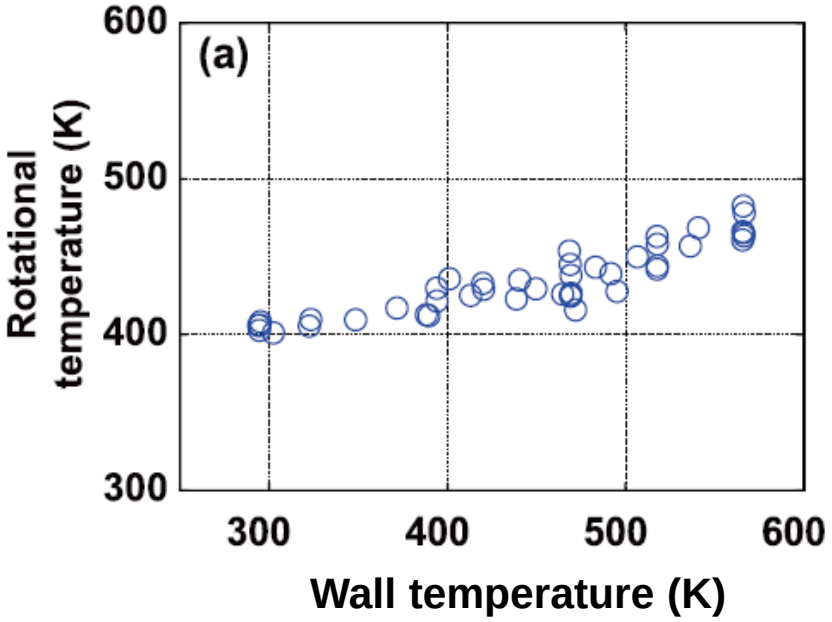


Dependence of rotational states distribution of plasma near wall on wall temperature

Simulation results using wall model + neutral transport for JA-DEMO



Actual rotational temperature by spectroscopic measurement in GAMMA10



A. Terakado, et al., Plasma Fusion Res. 13, 3402096 (2018).

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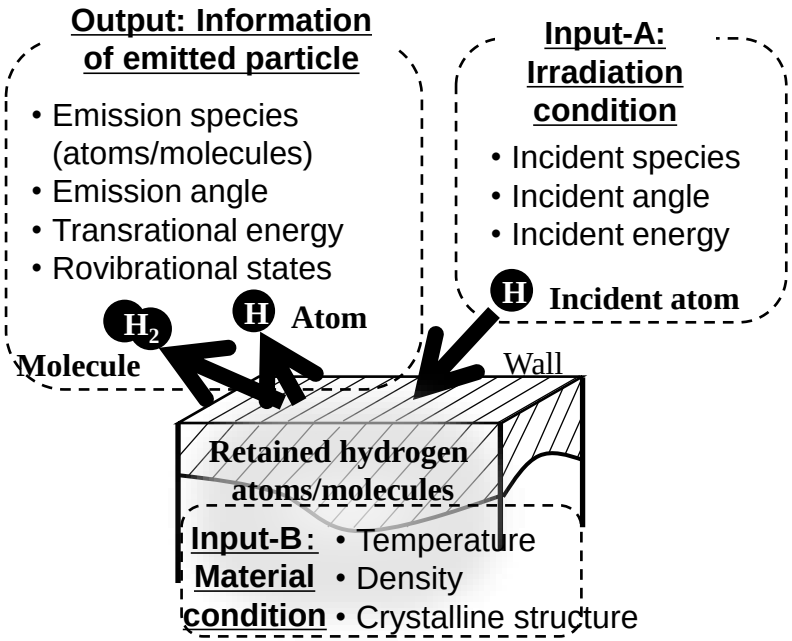
Application of Machine Learning (ML) to Hydrogen Recycling Model



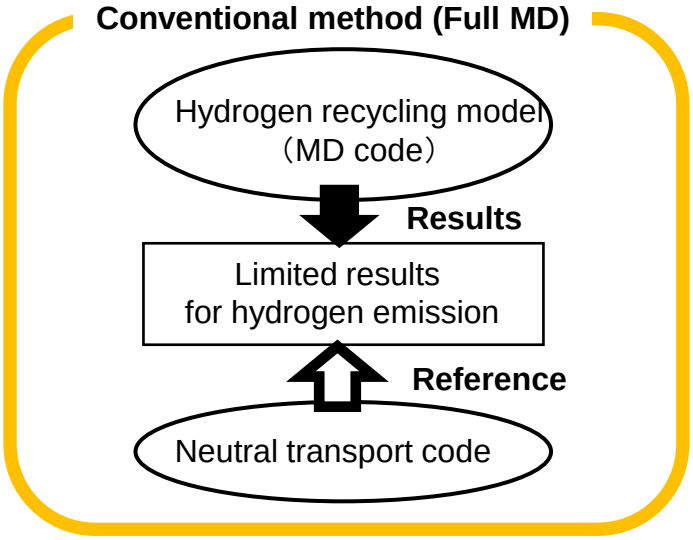
Changes in particle emission distribution

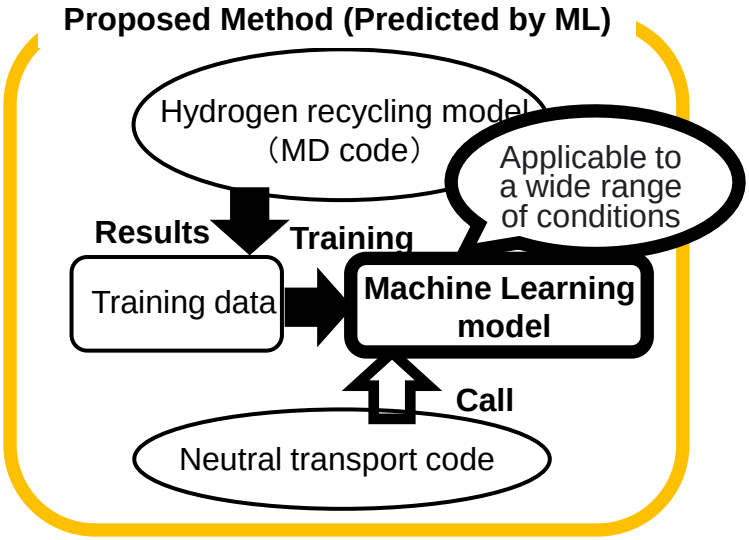
Plasma condition
- Density: n_e
- Elec. temp.: T_e
- Ion temp.: T_i

Interaction

Wall condition
- Mater. temp.: T_m
- Particle density: ρ
- Crystl. struct.

Changes in incident energy, flux, etc.

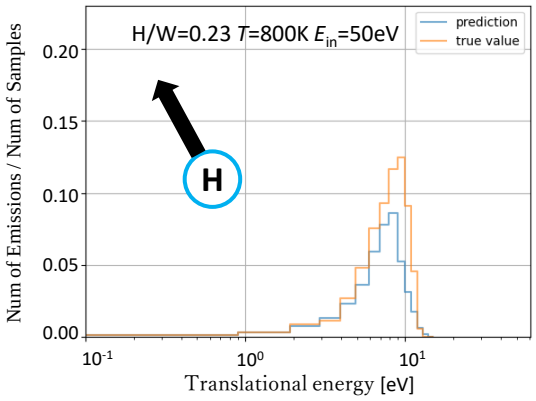




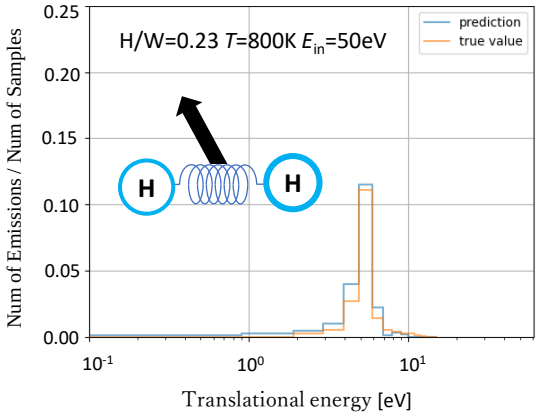
Prediction results of release distribution

S. Saito, *et al*., "*Machine learning-based hydrogen recycling model for predicting rovibrational distributions of released molecular hydrogen on tungsten materials via molecular dynamics simulations*", Nuclear Materials and Energy. **43** 101942 (2025).

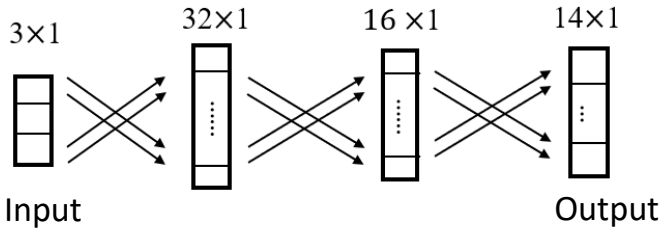
Translational energy of H atoms



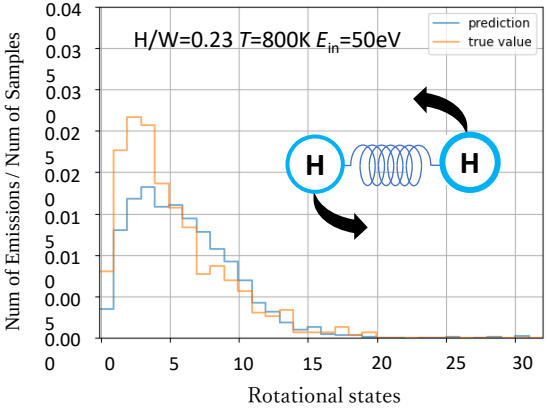
Translational energy of H_2 molecules



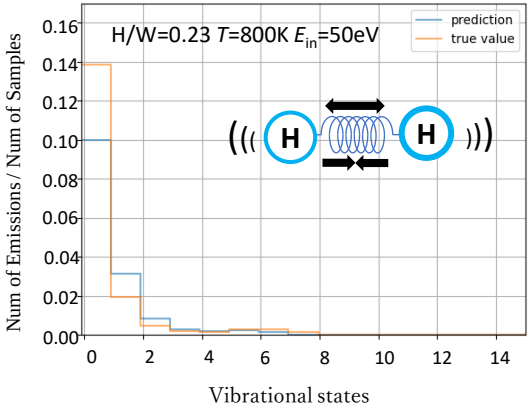
Network models for prediction of translational energy of H aotms



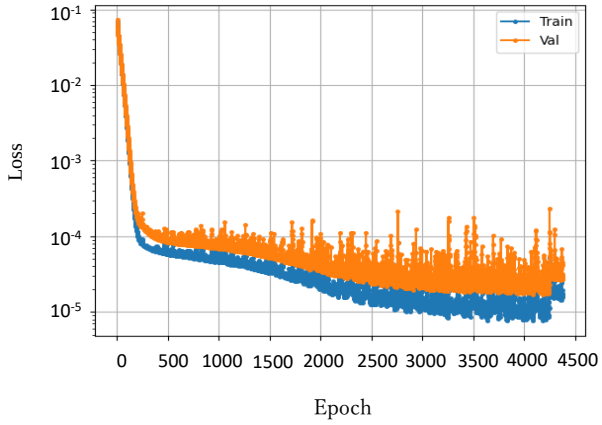
Rotational states of H_2 molecules



Vibrational states of H_2 molecules



Evolution of Loss function (MSE)



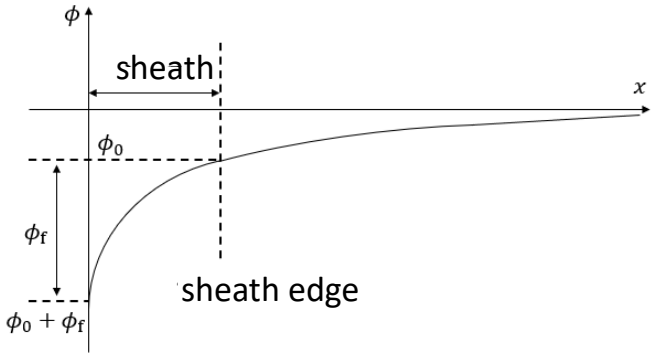
Consideration of incident energy distribution (Shifted-Maxwellian)

Distribution of incident energy E_{in} considering acceleration by sheath （Shifted-Maxwellian）

$$f(T_{\mathrm{i}}, T_{\mathrm{e}}: E_{\mathrm{in}}) = \frac{2}{\sqrt{\pi}} \cdot \frac{1}{(T_{\mathrm{i}})^{\frac{3}{2}}} \cdot \sqrt{E_{\mathrm{in}} - e(\phi_{\mathrm{f}} + \phi_0)} \cdot \exp\left(-\frac{E_{\mathrm{in}} - e(\phi_{\mathrm{f}} + \phi_0)}{T_{\mathrm{i}}}\right)$$

$$e(\phi_{\mathrm{f}} + \phi_0) = \left\{\frac{1}{2}\ln\left[\left(2\pi\frac{m_{\mathrm{e}}}{m_{\mathrm{i}}}\right)\left(1 + \frac{T_{\mathrm{i}}}{T_{\mathrm{e}}}\right)\right] + \frac{1}{2}\right\} T_{\mathrm{e}}$$

T_{i}, T_{e} : Ion/Electron temperature, m_{i}, m_{e} : Ion/Electron mass

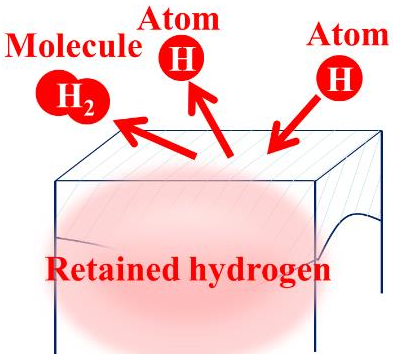


Integrate the output distribution of the machine learning model according to the distribution f of the incident energy E_{in}

$$\Phi_x^{\mathrm{M}}(\Lambda, T_{\mathrm{m}}, E_{\mathrm{in}}: x) = \int_0^{\infty} f(T_{\mathrm{i}}, T_{\mathrm{e}}: E_{\mathrm{in}}) \boldsymbol{\Phi(\Lambda, T_{\mathrm{m}}, E_{\mathrm{in}}: x)} \mathrm{d}E_{\mathrm{in}}$$

Machine learning model for the distribution of *x*

x*: Translational energy *E* / Rotational state *J* / Vibrational state *v

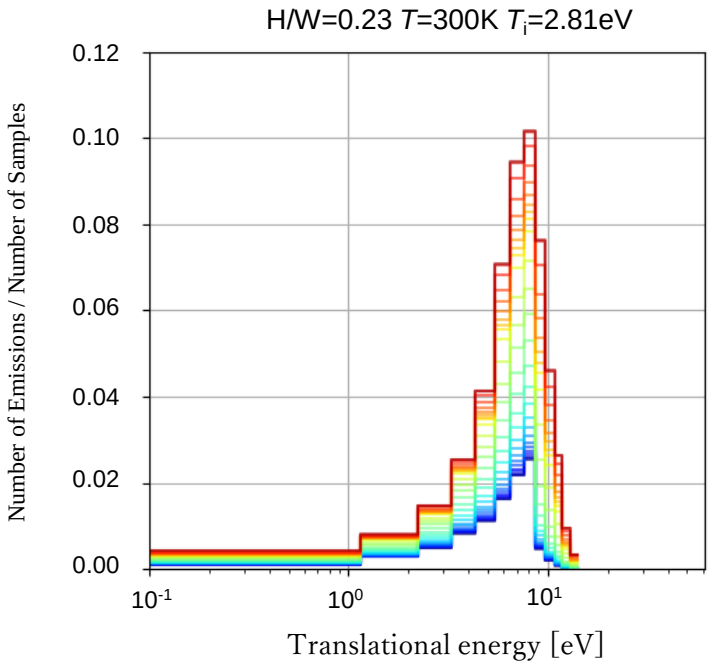


Λ: H/W

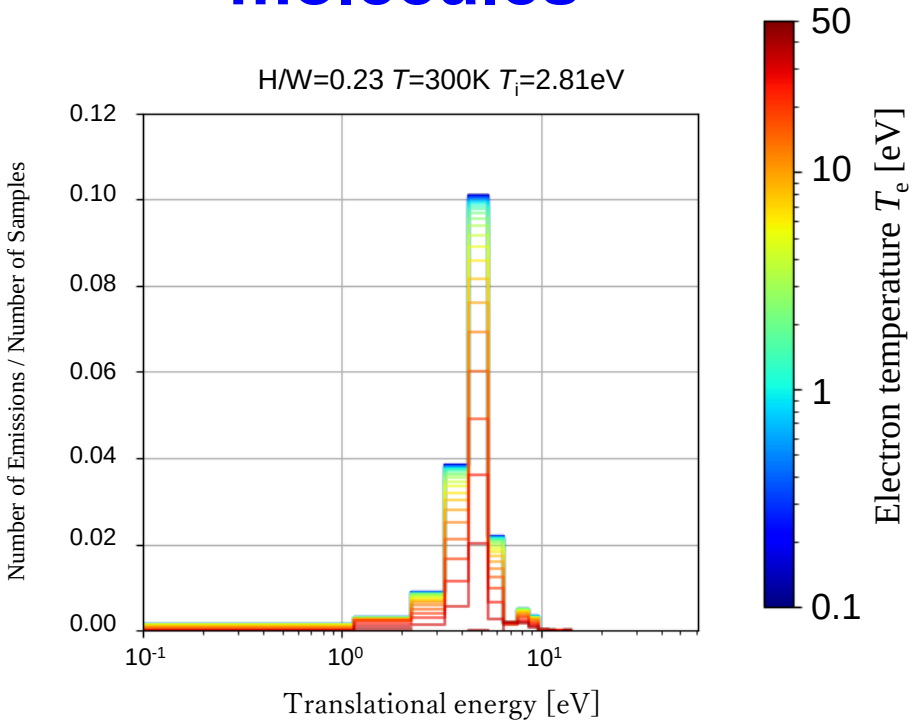
T_{m}: Material temperature

Translational energy distribution of recycled **atoms** and **molecules** considering Maxwell distribution

atoms



molecules



The higher the electron temperature and the deeper the sheath, the greater the amount of atoms emitted.

The lower the electron temperature and the shallower the sheath, the greater the amount of molecular emission.

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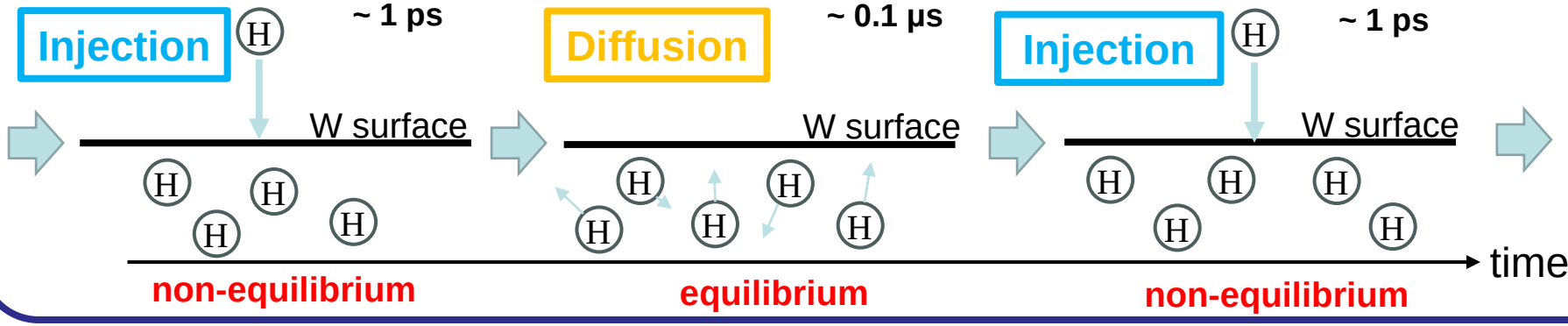
5. Future work: towards advanced wall modeling

Attempt at a Deep Learning Assisted kMC-MD Hybrid Method

Objective: Simulation of hydrogen atom accumulation due to continuous injection

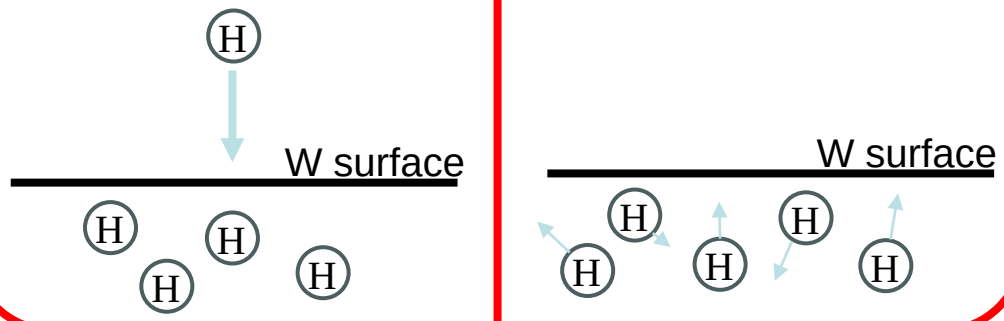


Comparison of methods

- Molecular dynamics (MD)
- kinetic Monte Carlo (kMC)

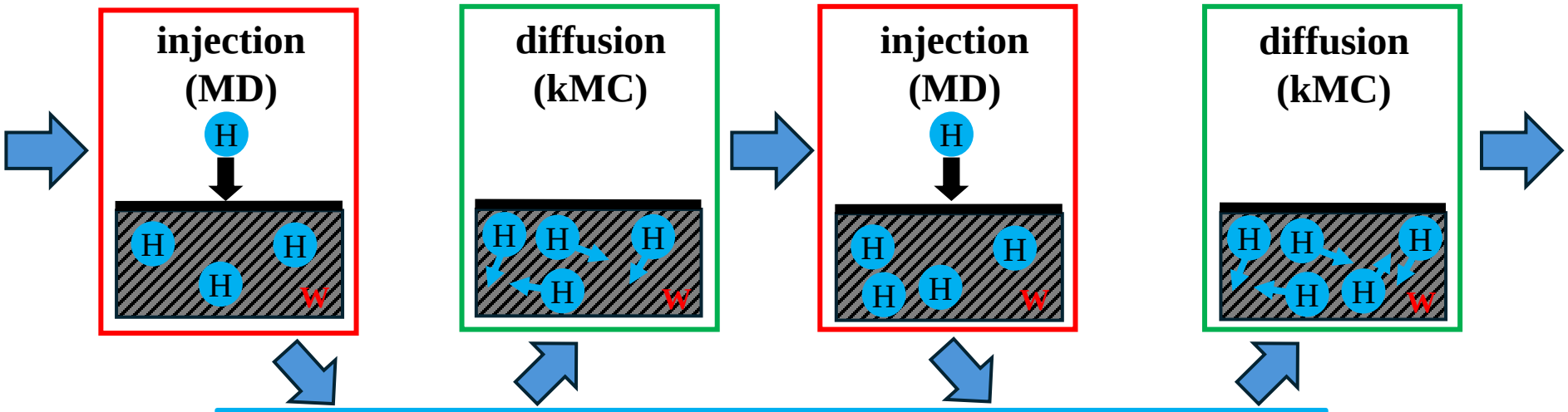
	Comp. Cost	Sim. in Non-Eq. States
MD	×	○
kMC	○	×

Hybrid simulation method



Purpose and method

Hybrid method has the problem that it needs considerable computation cost for the calculation of the migration barrier and trapping site required for kMC calculation.



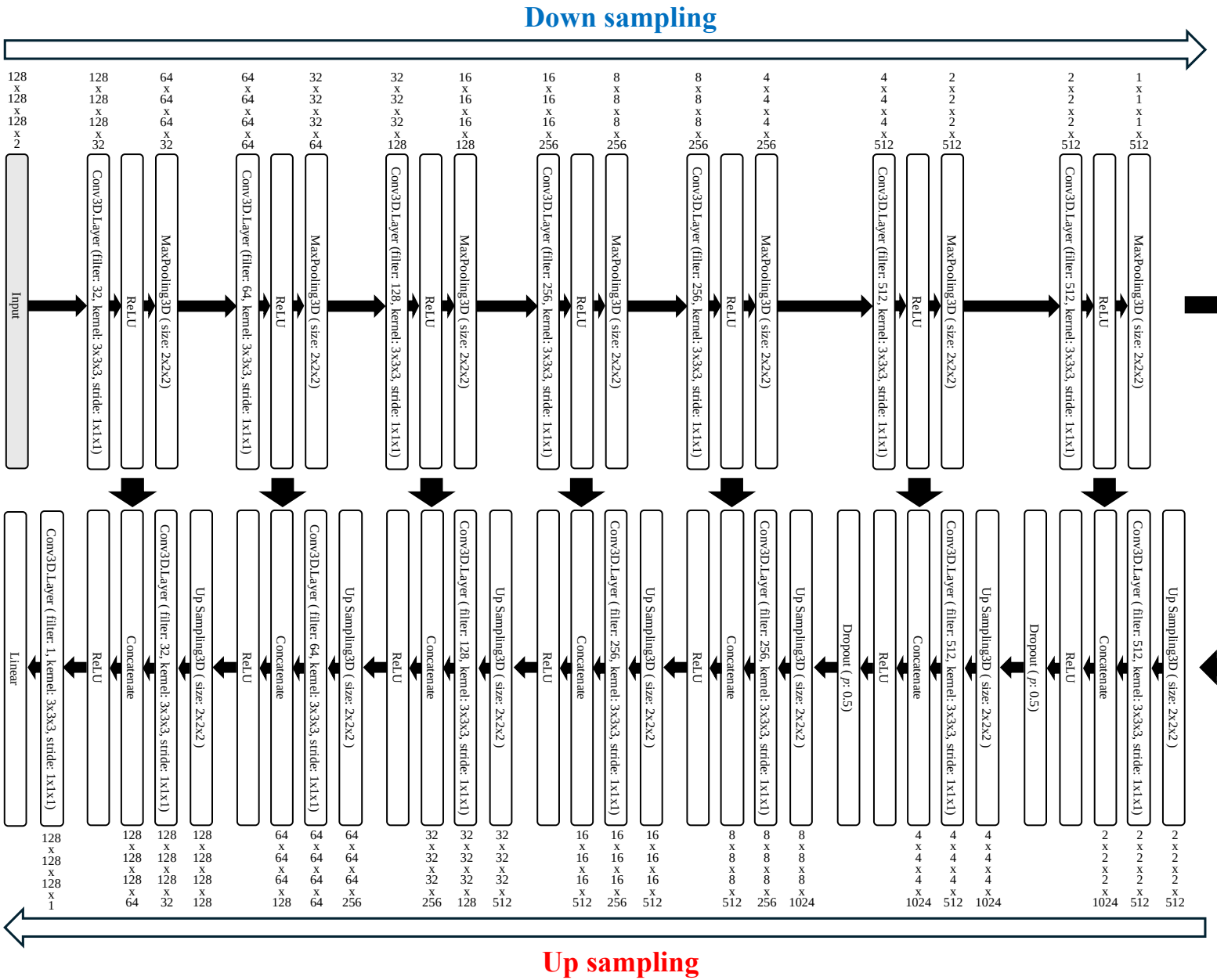
Predicting the following three values by deep learning models :

① 3D potential energy distribution } **Today's topic**

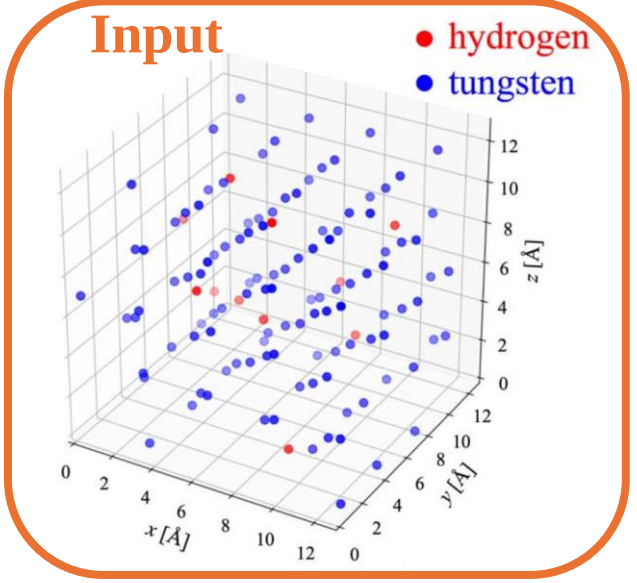
② Migration barrier

③ Minimum potential point (trapping site) } **Under development**

Network model (Generator)



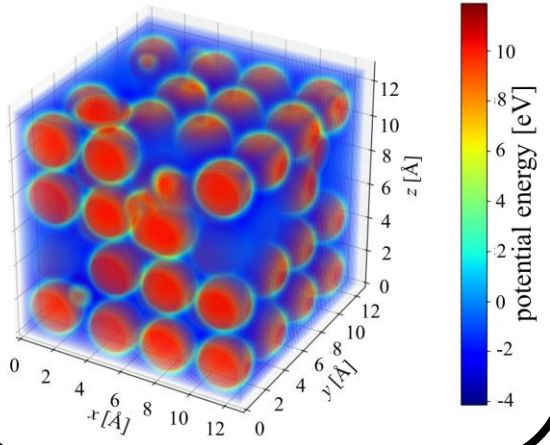
Results of prediction of 3D potential energy distribution



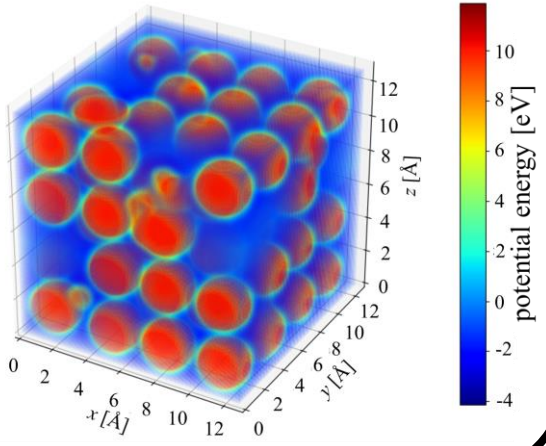
EAM potential
4 hours
by 1 CPU(1 core)

DL model
0.2 second by
1 CPU(1 core) + 1 GPU

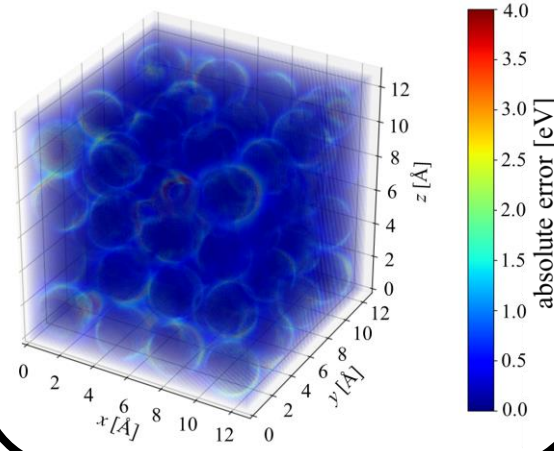
Ture values



Predicted values



Absolute error



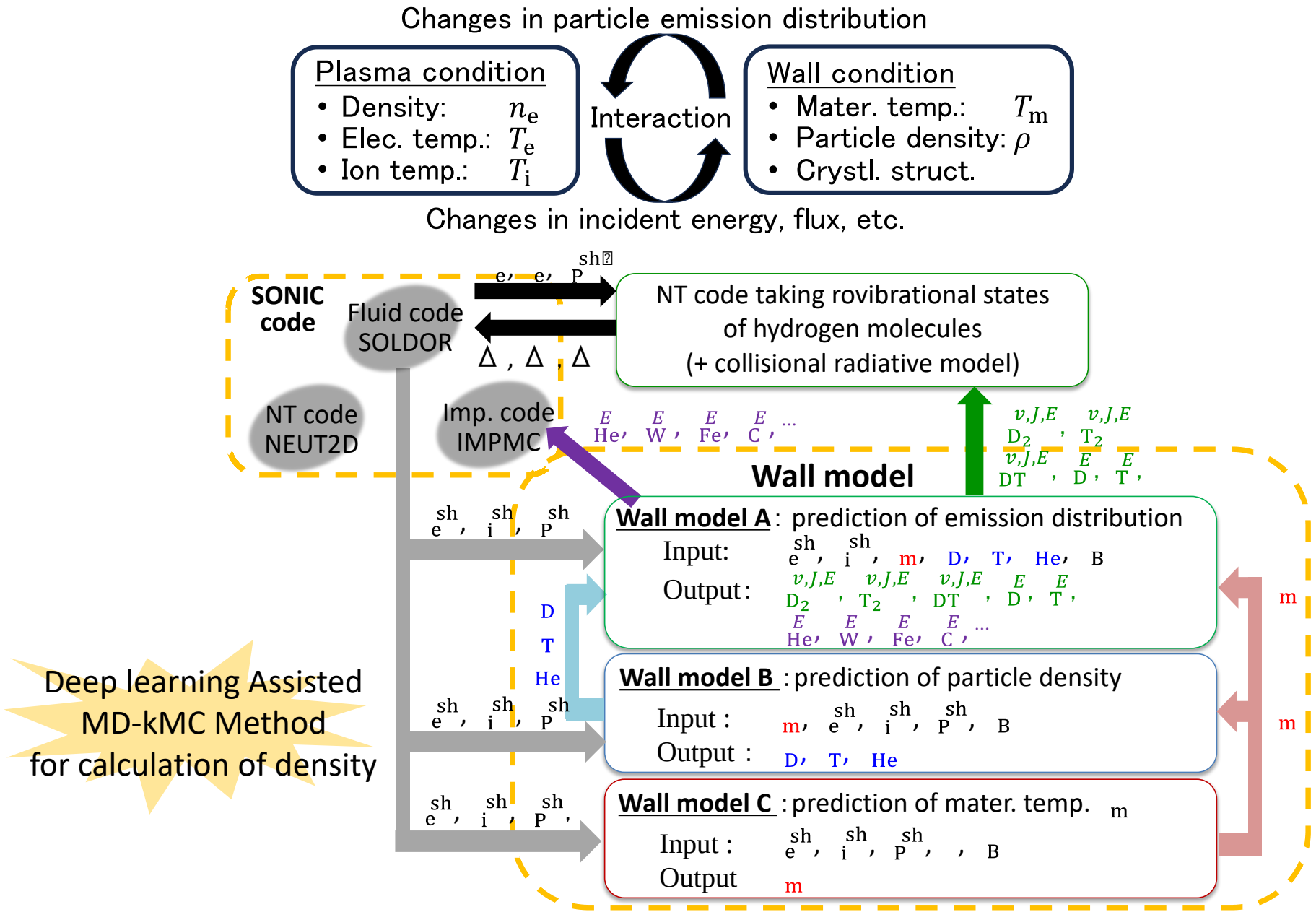
The accuracy is good based on the comparison between the true and predicted values

S. Saito, *et al*., "*Deep learning model for predicting the spatial distribution of binding energy from atomic configurations*", Japanese Journal of Applied Physics, **63**, (2024).

Contents

1. Background
2. Molecular dynamics simulation of hydrogen recycling on tungsten wall
3. Integration with fluid codes and neutral transport simulation
4. Machine learning approaches for the wall model
    1. Prediction model for emission distribution
    2. Deep learning assisted kMC-MD hybrid simulation
5. Future work: towards advanced wall modeling

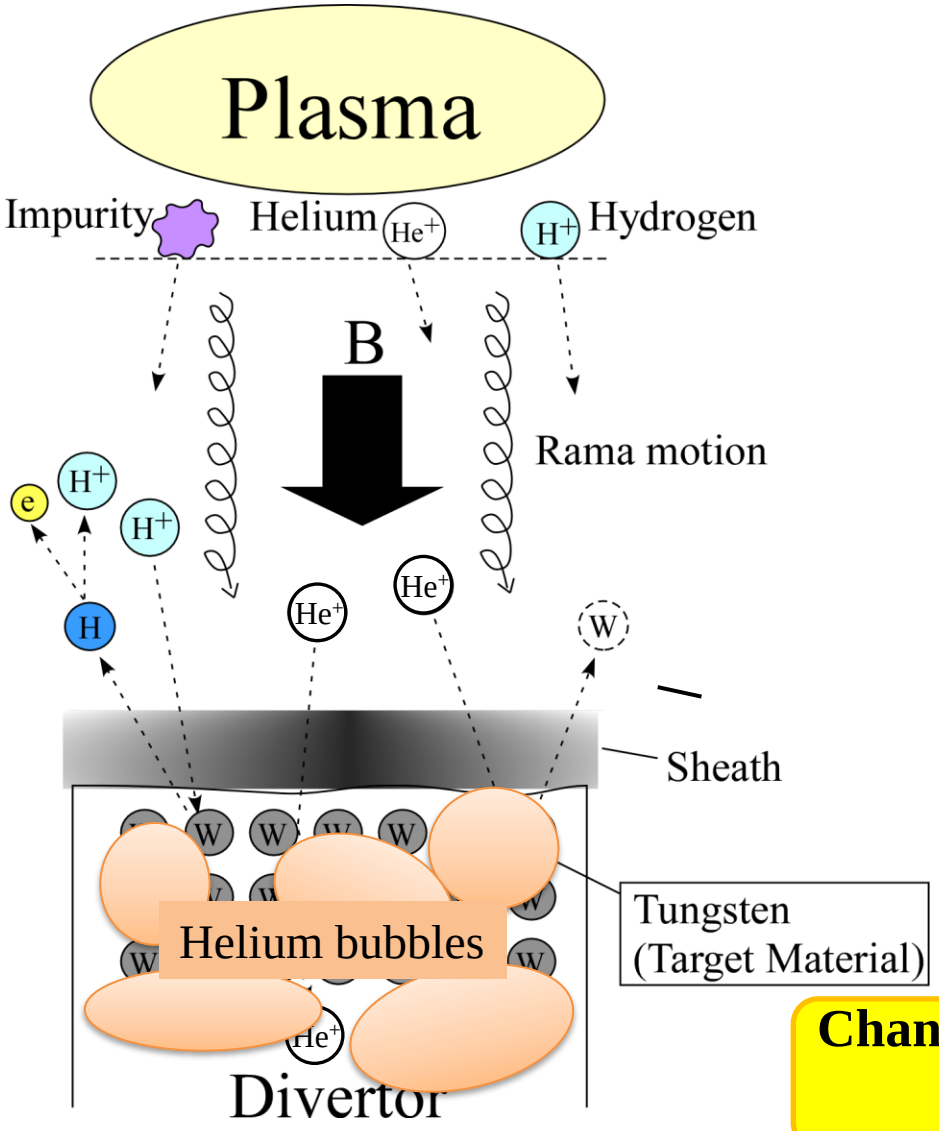
Future work: towards advanced wall modeling

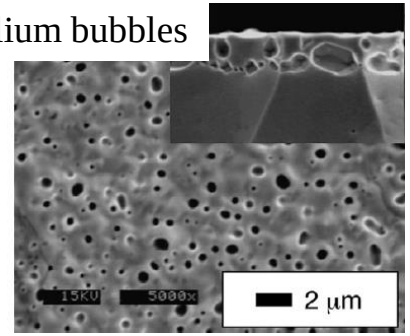


Summary

- Hydrogen recycling on tungsten walls was investigated using MD simulations.
- Emission distributions of rovibrational states of recycled hydrogen were predicted using machine learning techniques.
- The developed wall model was integrated with the SONIC code and neutral transport simulations.
- Future plan: We will develop a deep learning-assisted kMC–MD hybrid method to generate training data for machine learning models that predict particle density. The model will provide input for emission distribution predictions and enable to solve the dynamical interaction between plasma and wall.

Radiation damage to walls (helium bubbles)





N. Ohno, et. al., J. Nucl. Mater. 363 (2007) 1153

retention

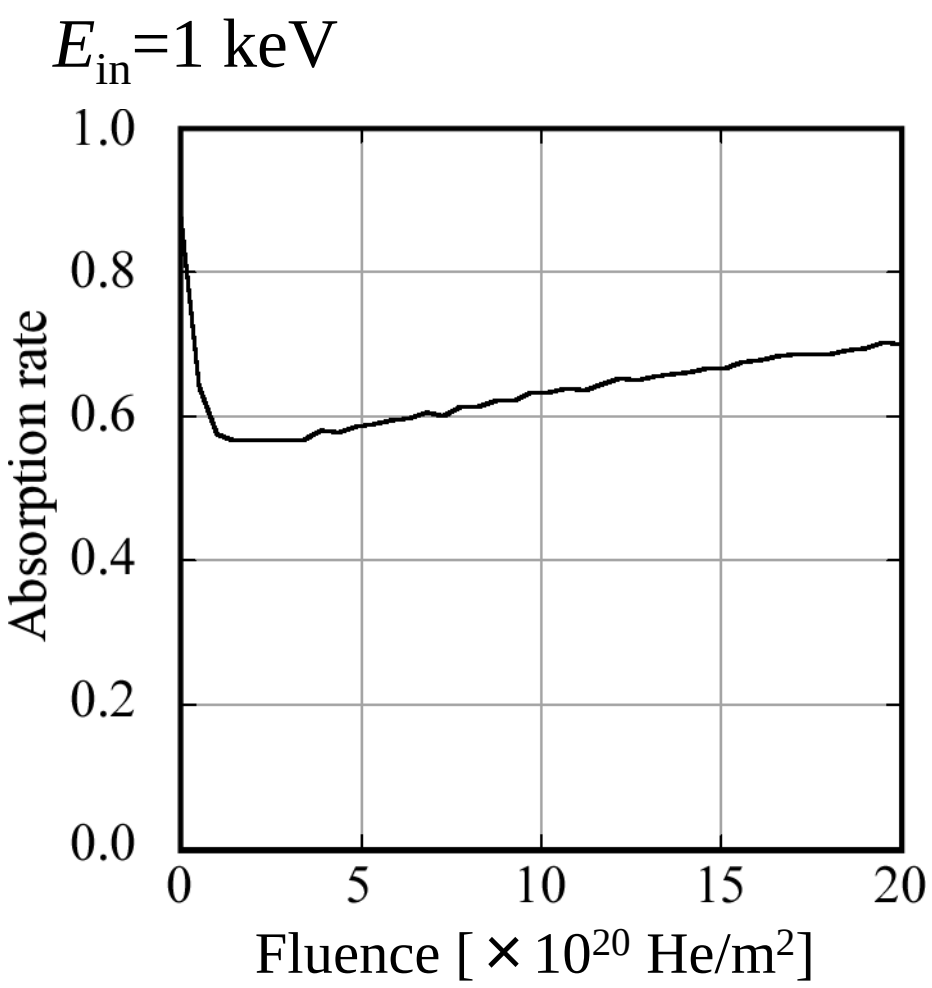
Accumulate of the Plasma particles in the material

sputtering

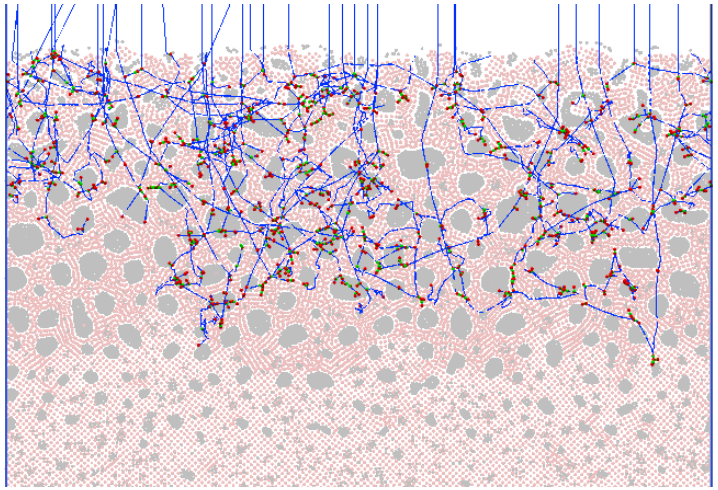
Emission of material atoms by collisions with plasma particles

Changes in the material surface structure (generation of helium bubbles)

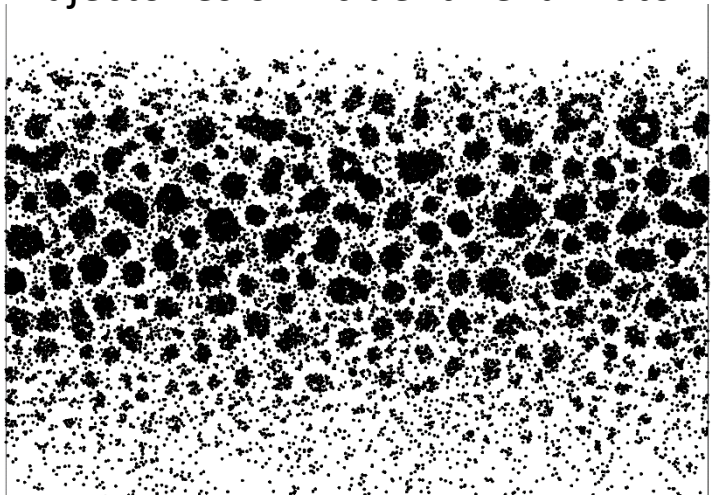
Time evolution of absorption rate by helium irradiation



S. Saito, et al., JJAP. 55 (2016) 01AH07
S. Saito, et al., proc. JSST2017 (2017)
S. Saito, et al., JJAP. 56 (2017) 01AF04



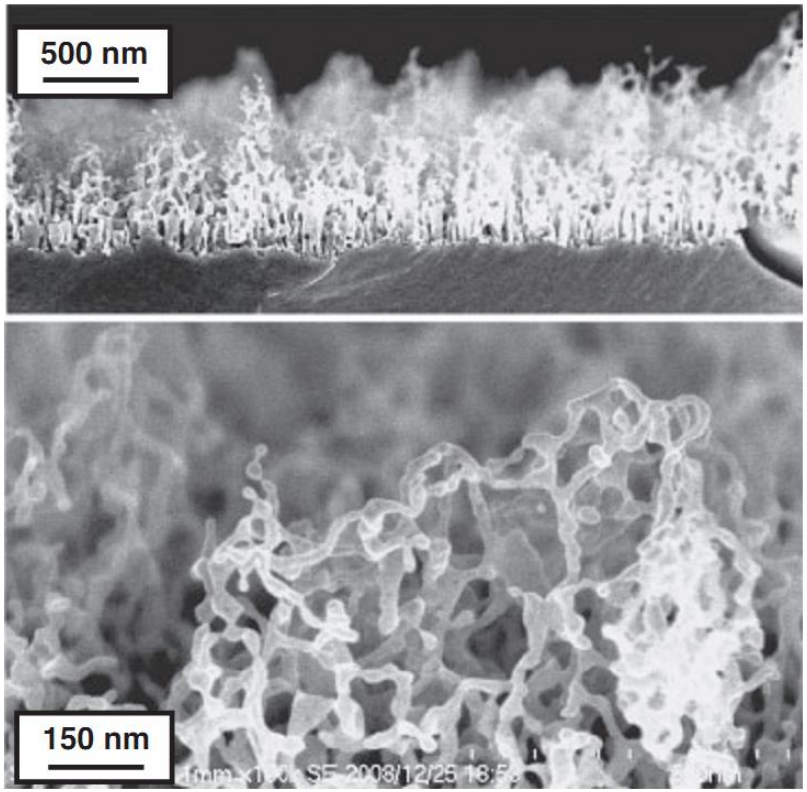
Trajectories of incident helium atoms



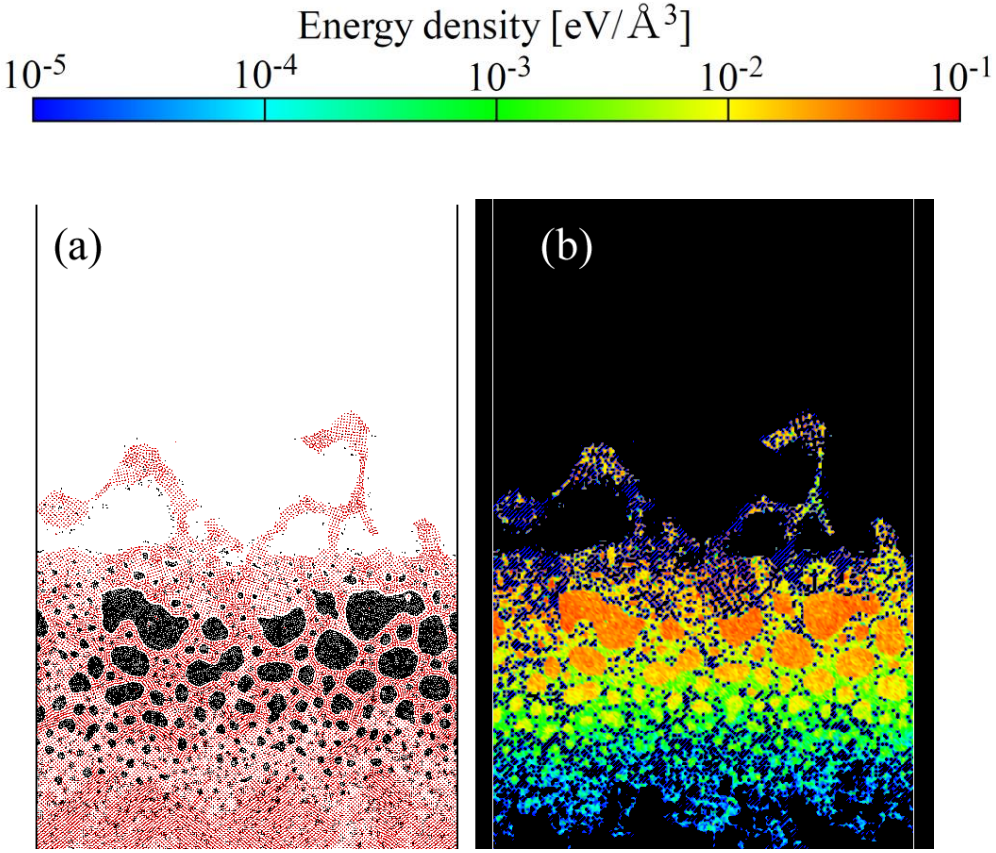
Plot of stopping positions of incident helium atoms

Energy absorption on the fuzz structured surface

Fuzz structure of tungsten surface formed by helium plasma exposure.

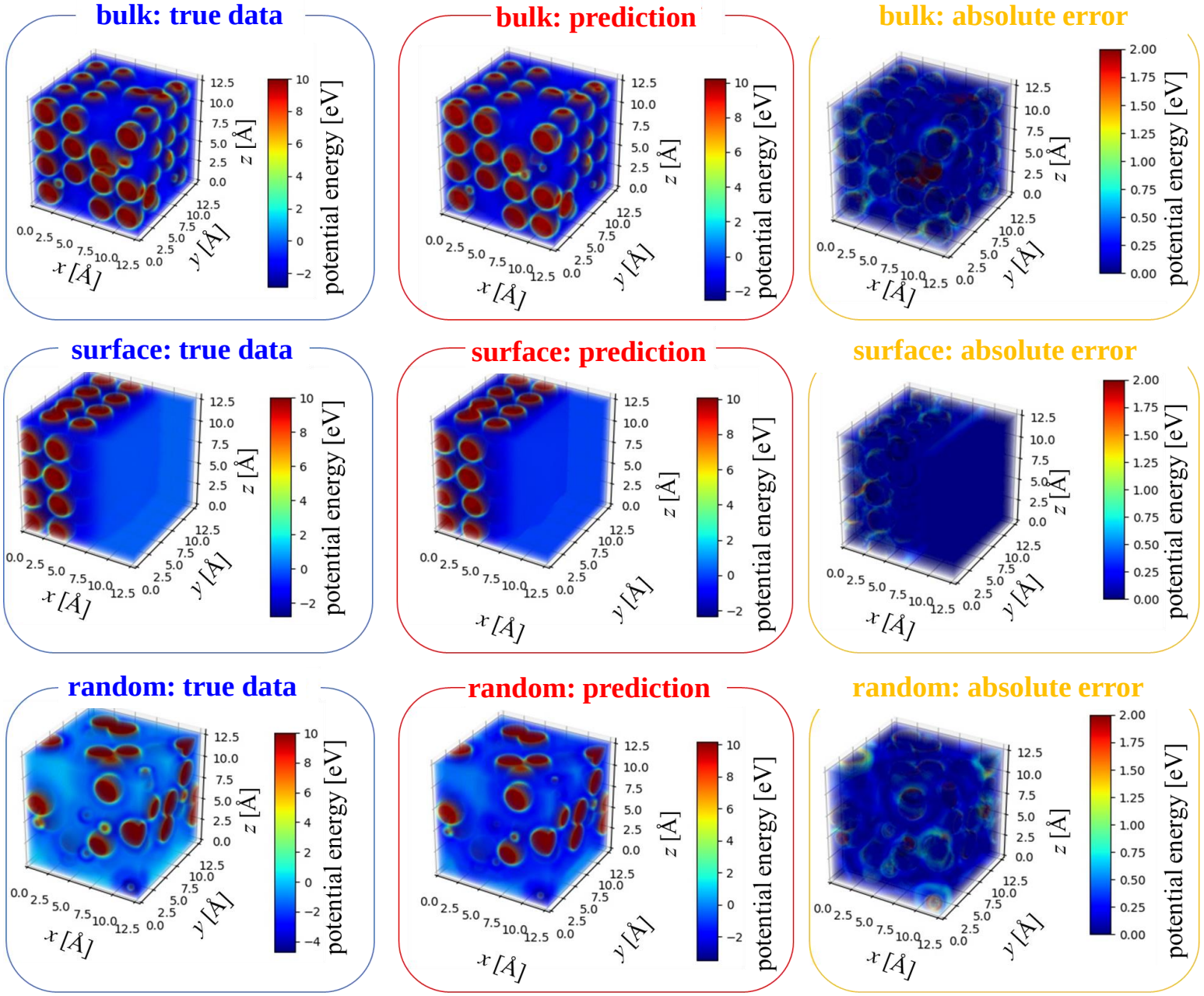


S. Kajita, et al., JJAP. 50 (2011) 08JG01

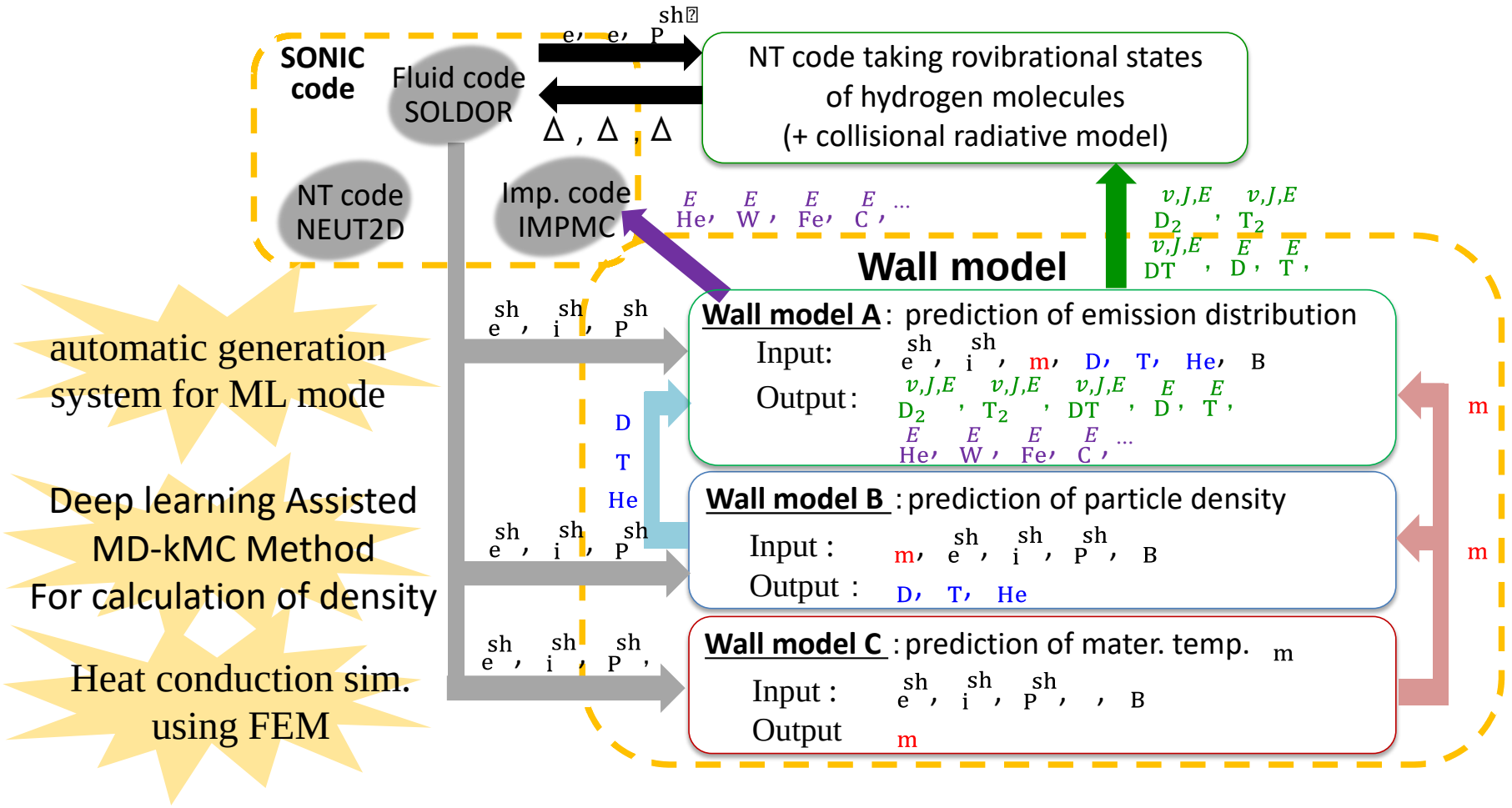


S. Saito, et al., JJAP. 55 (2016) 01AH07
S. Saito, et al., proc. JSST2017 (2017).
S. Saito, et al., JJAP. 56 (2017) 01AF04

Results of prediction of 3D potential energy distribution



S. Saito, *et al*., Jpn. J. Appl. Phys. 63 9SP03 (2024).

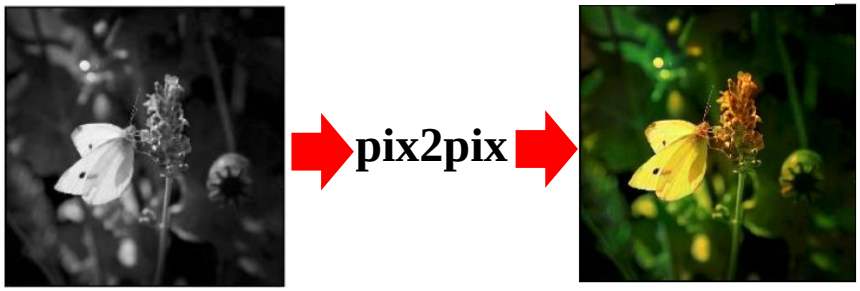


n_e, T_e :	Electron density and temperature of edge plasma
$T_e^{sh}, T_i^{sh}, \Gamma_P^{sh}$:	Electron temperature, ion temperature, and flux to the wall at the sheath edge
$\Delta n, \Delta\boldsymbol{\pi}, \Delta\epsilon$:	Increments in density, momentum, and energy of ions resulting from neutral transport
T_m :	Wall temperature
θ_B :	Incident angle of magnetic field lines to the wall
$\rho_D, \rho_T, \rho_{He}$:	Deuterium, tritium, and helium densities in the wall
$f_x^{v,J,E}$:	The distribution of rovibrational states, and translational energy of released molecule x

cf. pix2pix

Generative adversarial network (GAN) for 2D image to 2D image conversion

Example: Converting grayscale image to a color image



Phillip Isola, Jun-Yan Zhu, Tinghui Zhou, Alexei A. Efros,
Image-to-Image Translation with Conditional Adversarial Networks
https://arxiv.org/pdf/1611.07004.pdf

Overview of GAN

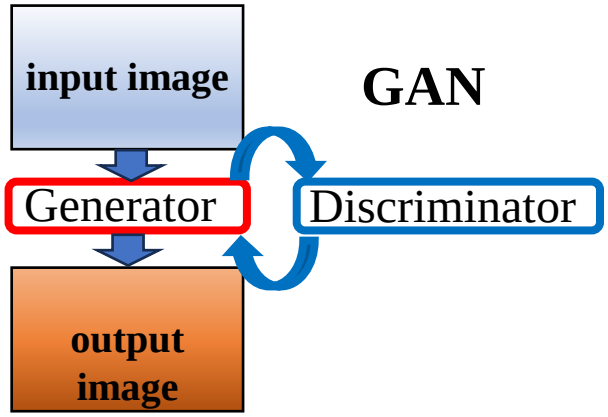
GAN consists of two networks: a generator and a discriminator.

- **Generator**

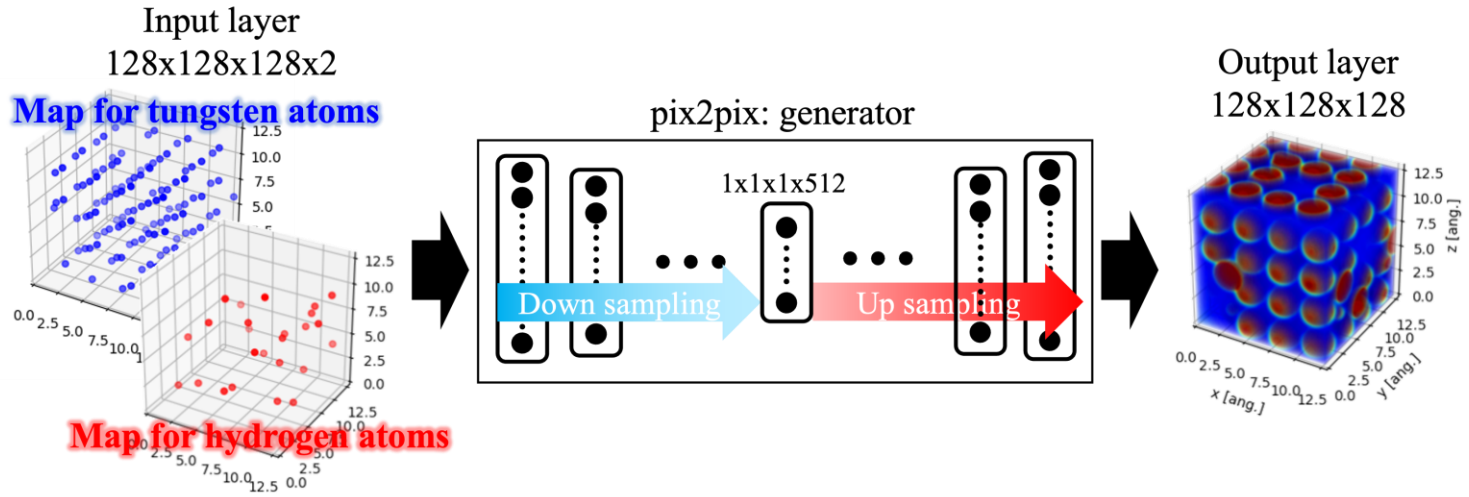
Output the desired image from the input image.

- **Discriminator**

Judge whether the image is generated or real one.



Usage of deep learning in kMC



Expansion of pix2pix from 2D to 3D

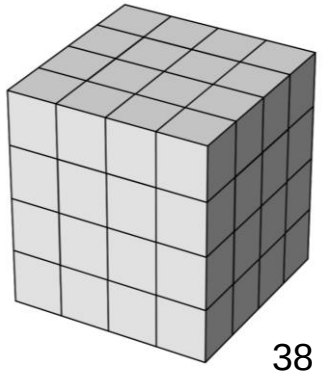
2D image

- Pixels (arranged in 2D array)
- Pixel value represents the intensity of the pixel.

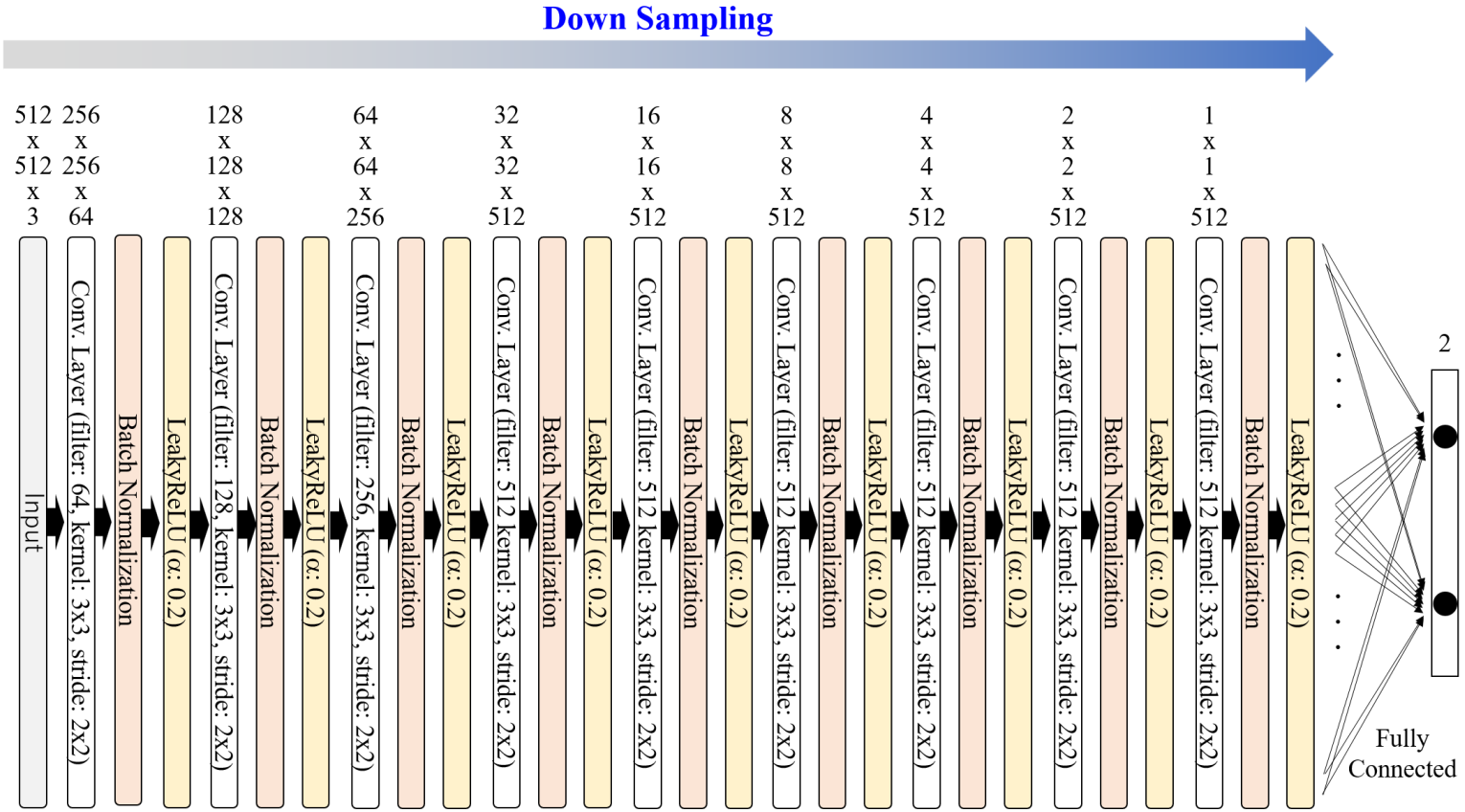
255	255	0	0	0
255	255	0	0	0
255	255	100	100	100
255	255	100	100	100

3D image

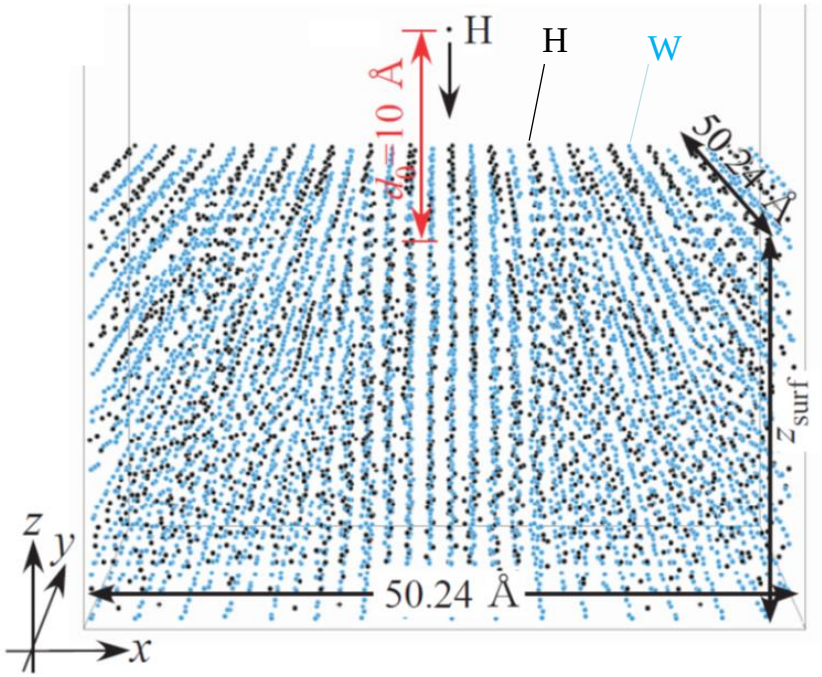
- Voxels (arranged in 3D array)
- Voxel value represents the potential energies.



Structure discriminator



Generation of training data by MD simulation



Simulation Condition

- Target material: bcc tungsten containing hydrogen
- Boundary condition: Periodic boundary condition (*x* and *y* directions)
- Atomic interaction: EAM potential
- Heat bath: Langevin thermostat
- Incoming atom: Hydrogen atom
- Number of incident atoms: 1 atom
- Simulation time: 1ps

Training Data

- H/W (Λ): 0.1, 0.23
- Material temperature (T_m): 300, 600, 1000 [K]
- Incident energy (E_{in}): 0.1, 1, 10, 100 [eV]

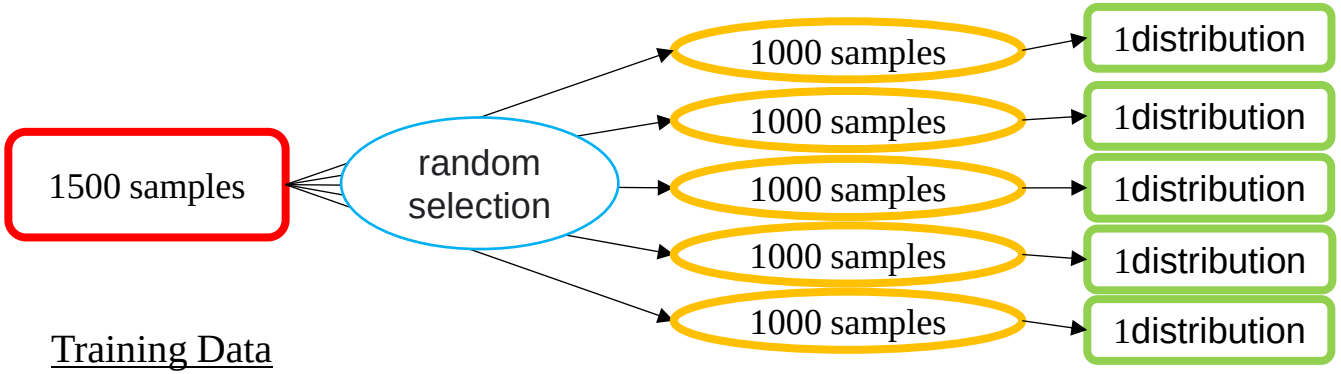
2(H/W) × 3(temperature) × 4(incident energy) = 24 patterns

Test Data

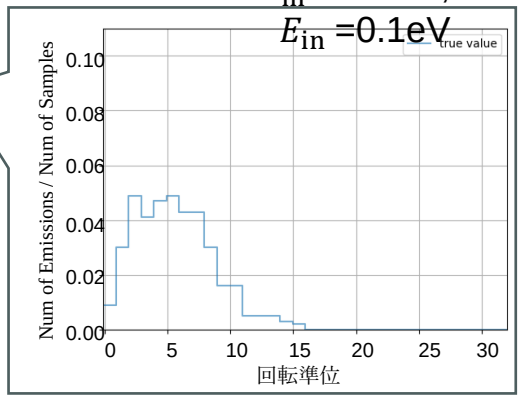
- H/W (Λ): 0.23
- Material temperature (T_m): 400, 800 [K]
- Incident energy (E_{in}): 5, 50 [eV]

2(temperature) × 2(incident energy) = 4 patterns

Machine Learning Model



Example: Λ =0.23, T_m =1000K, E_{in} =0.1eV



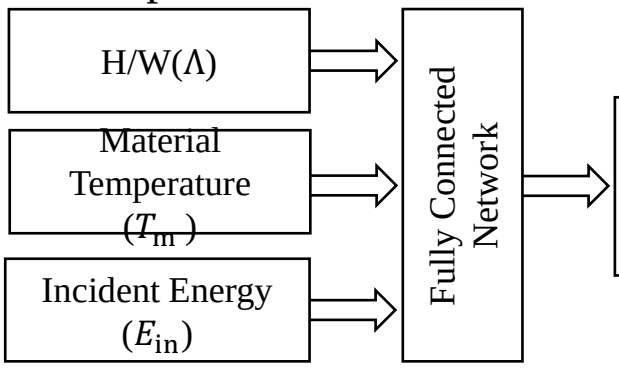
Training Data

2(H/W) × 3(temperature) × 4(incident energy) = 24 patterns

→ 24 × 5(random selections) = 120 training data

Training Data

Input



Output

1. Distributions of translational energy of emitted H atoms
2. Distributions of translational energy of emitted H_2 molecules
3. Distributions of rotational states of emitted H_2 molecules
4. Distributions of vibrational states of emitted H_2 molecules

Direct prediction model for emission distribution considering Maxwellian distribution

Emission distribution for monochromatic incident energy

Input: Λ , T_{m}, E_{in}

Integration with Maxwellian distribution

Emission distribution considering Maxwellian distribution

Input: Λ , T_{m}, T_{i}, T_{e}

Prediction by machine learning

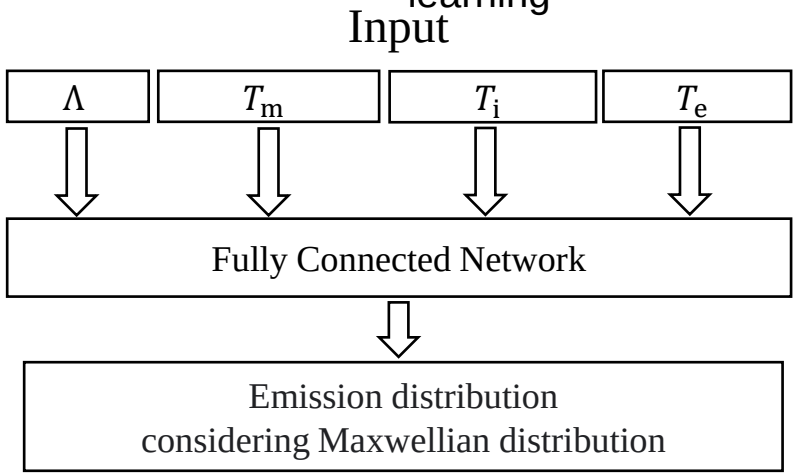
Emission distribution considering Maxwellian distribution

合計: 11664

80%

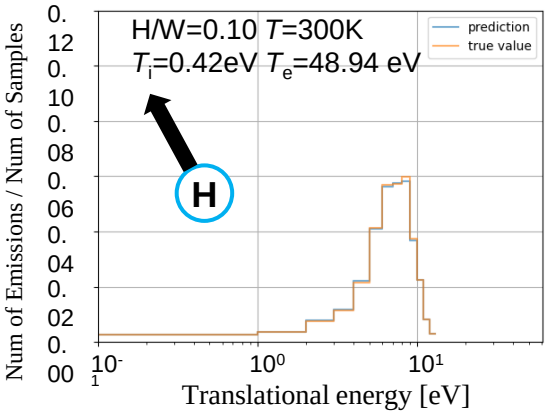
20%

Training Data	Test Data
9331	2333

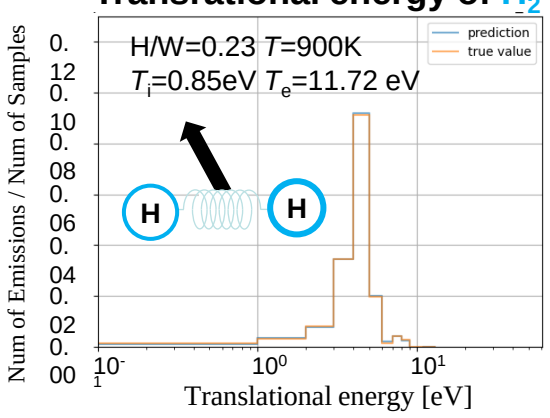


Result of prediction

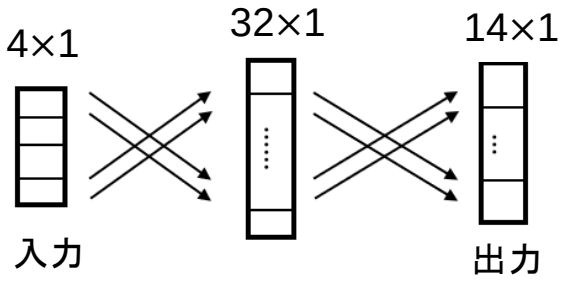
Transrational energy of H



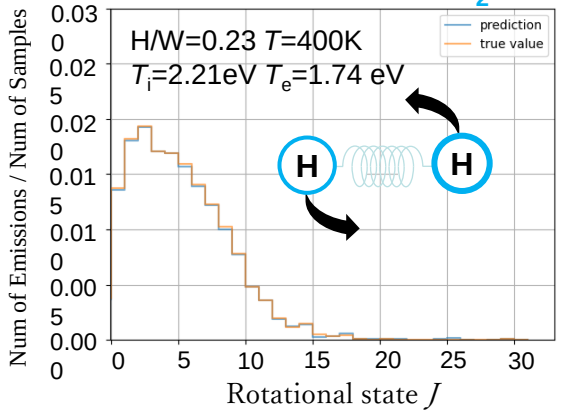
Transrational energy of H_2



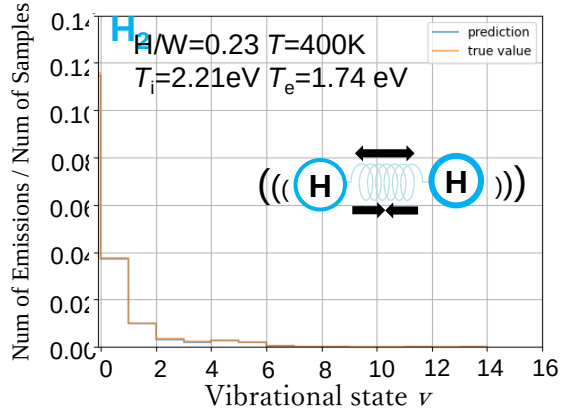
Atom translational energy distribution prediction model



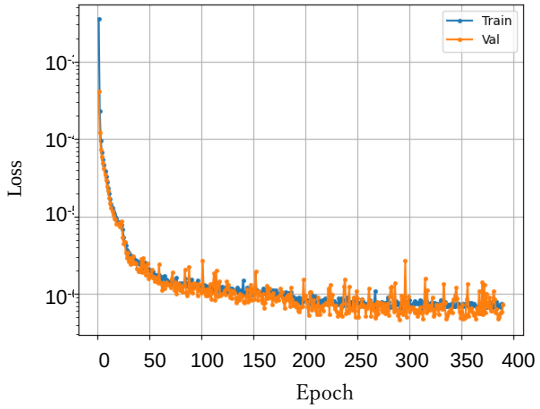
Rotational state of H_2



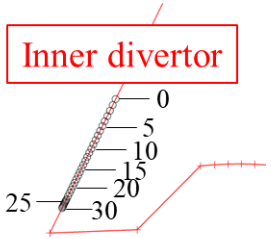
Vibrational state of H_2



Atom translational energy distribution Prediction model loss function (MSE)



Energy absorption due to excitation of rovibrational states



$$\Delta E_{\mathrm{e}} = \sum_{p,q} C_{\mathrm{e}}(T_{\mathrm{e}}: p,q) n(p) n_{\mathrm{e}} \, \Delta E(p,q)$$

$$\Delta E_{\mathrm{H}^+} = \sum_{p,q} C_{\mathrm{H}^+}(T_{\mathrm{e}}: p,q) n(p) n_{\mathrm{e}} \, \Delta E(p,q)$$

$$\Delta E_{\mathrm{H}} = \sum_{p,q} C_{\mathrm{H}}(T_{\mathrm{e}}: p,q) n(p) n_{\mathrm{H}} \, \Delta E(p,q)$$

C_* : Excitation rate coefficient due to collision with *

p : Vibration/rotation level before collision

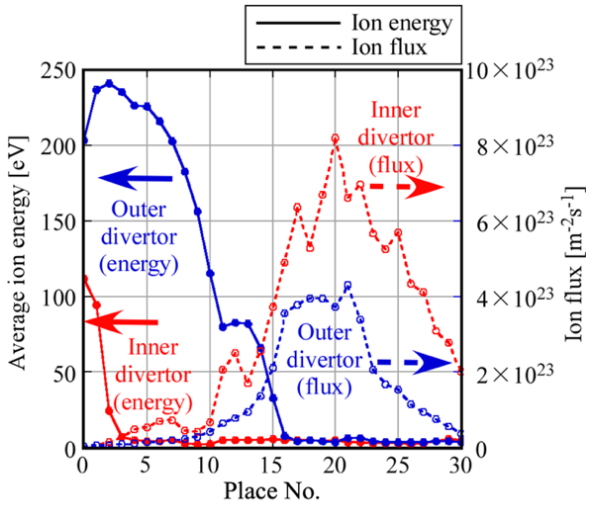
q : Vibration/rotation level after collision

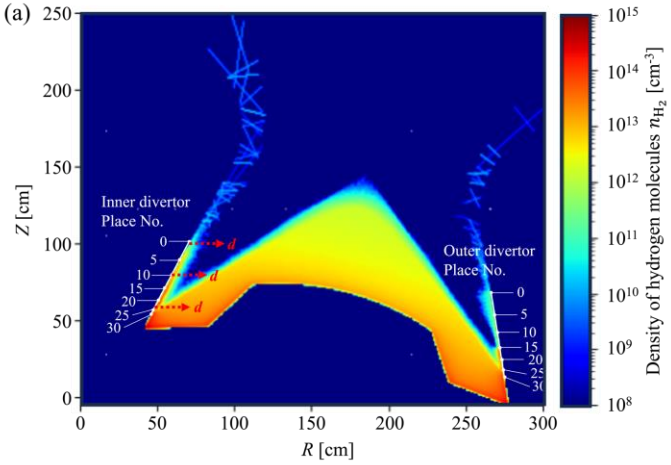
$\Delta E(p,q) \equiv E(q) - E(p)$,

$E(p)$: Energy eigenvalue at rovibrational state p

$n(p)$: Hydrogen molecule density at vibrational/rotational level p

Place No.	d [cm]	T_{e} [eV]	n_{e} [cm^{-3}]	$n_{\mathrm{H_2}}$ [cm^{-3}]	n_{H} [cm^{-3}]	ΔE_{e} [eV/(cm^3 s)]	ΔE_{H^+} [eV/(cm^3 s)]	ΔE_{H} [eV/(cm^3 s)]
1	2	13.0	1.3×10^{13}	2.9×10^{9}	4.6×10^{11}	1.9×10^{15}	2.9×10^{15}	3.1×10^{10}
10	2	1.9	1.8×10^{15}	1.2×10^{10}	2.5×10^{14}	1.9×10^{19}	1.2×10^{18}	2.7×10^{12}
23	2	2.3	2.8×10^{15}	4.3×10^{9}	3.2×10^{14}	1.7×10^{19}	1.0×10^{18}	4.1×10^{11}





$$\Delta E_{\mathrm{e}} = \sum_{p,q} C_{\mathrm{e}}(T_{\mathrm{e}}: p, q) n(p) n_{\mathrm{e}} \, \Delta E(p, q)$$

p : Vibration/rotation level before collision

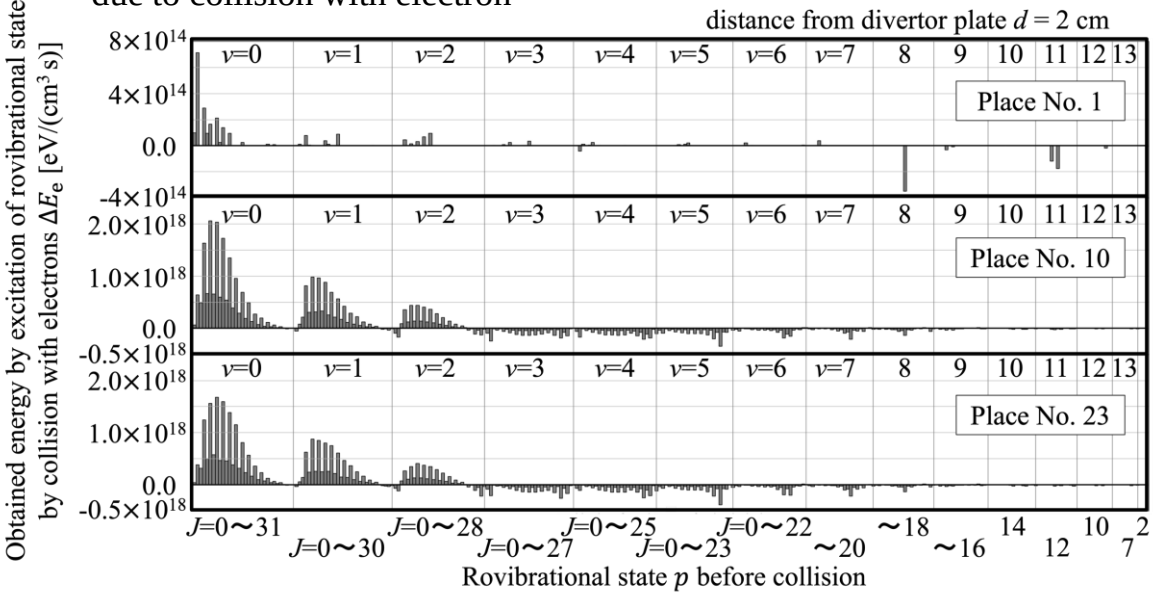
q : Vibration/rotation level after collision

C_{e} : Excitation rate coefficient due to collision with electron

$\Delta E(p, q) \equiv E(q) - E(p)$,

$E(p)$: Energy eigenvalue at rovibrational state p

$n(p)$: Hydrogen molecule density at vibrational/rotational level p



Calculation of vibrational state v and rotational state J of H_2 molecule

1. Calculate rotational state J from total angular momentum L of hydrogen molecule in center-of-mass coordinate system obtained from MD

$$L^2 = \hbar^2 J(J+1) \quad \Longleftrightarrow \quad J = \frac{1}{2}\left(\sqrt{1+4\left(\frac{L}{\hbar}\right)^2} - 1\right)$$

2. Calculate the total energy E in center-of-mass coordinate

Classical system:

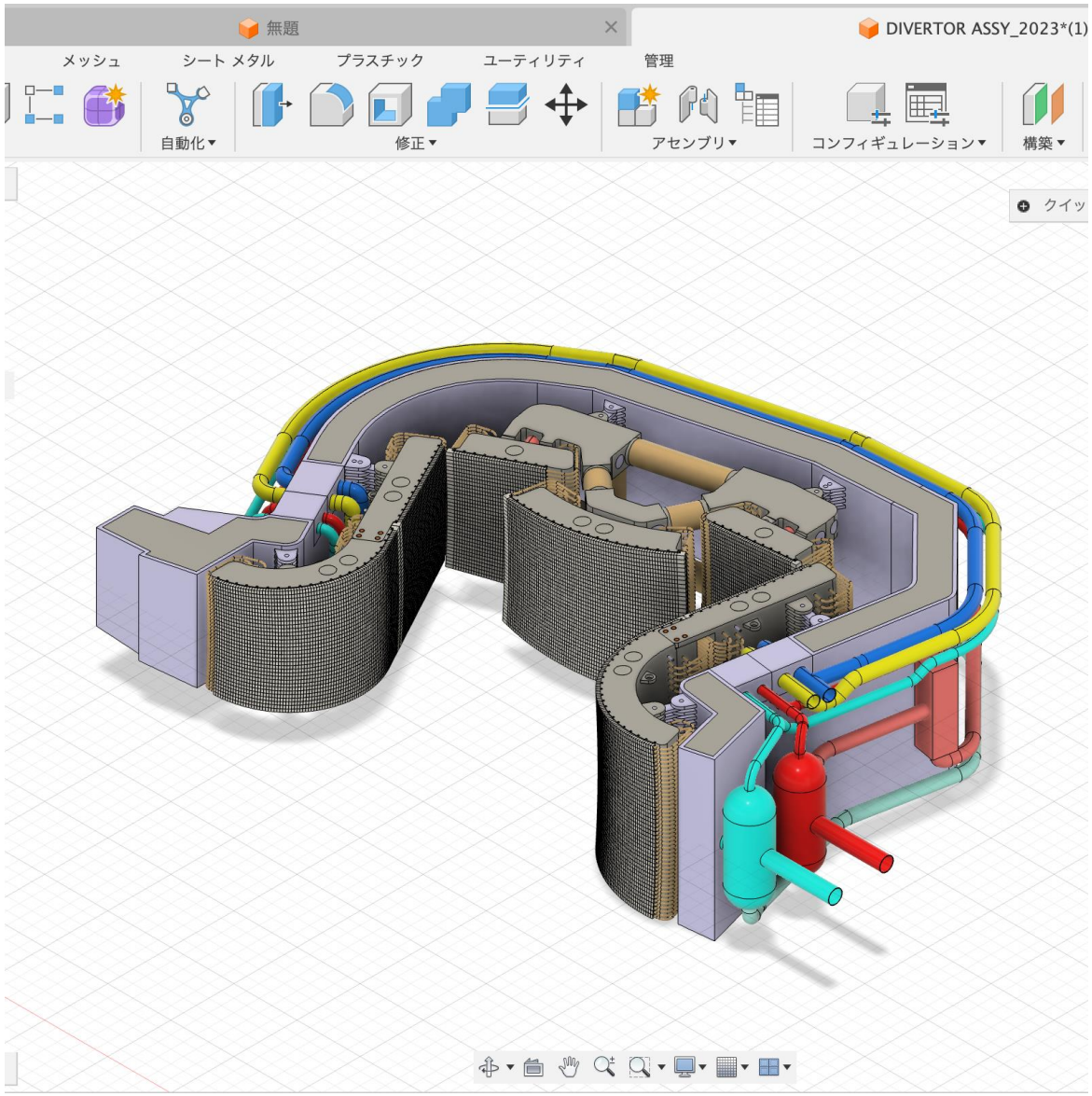
$$\frac{1}{2}\mu\left(\frac{dR}{dt}\right)^2 + U(R) + \frac{1}{2\mu}\left(\frac{L}{R}\right)^2 = E$$

R : Internuclear distance
μ : Reduced mass
$U(R)$: Potential function

3. Find the v closest to the values of J and E from the table of J, v and E pairs obtained by solving the Schrodinger equation in center-of-mass coordinate system.

Quantum system:

$$-\frac{\hbar^2}{2\mu}\frac{d^2\psi_v}{dR^2} + U(R)\psi_v + \frac{\hbar^2}{2\mu}\frac{J(J+1)}{R^2}\psi_v = E\psi_v$$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DIVERTOR ASSY_2023*(1)
メッシュ
シート メタル
プラスチック
ユーティリティ
管理
自動化
修正
アセンブリ
コンフィギュレーション
構築
クイッ