Development of Simulation Codes to Treat Hydrogen Molecule Processes in Divertor Plasma Region including Divertor Plate

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ABSTRACT

- Combining the neutral-transport (NT) code including the rovibrationally resolved collisional-radiative (CR) model with the molecular dynamics (MD) simulation, we clarify the influence of the divertor plate accurately on the spatial distribution of hydrogen atoms and molecules (H, H_2) in the divertor plasma region.
- Due to the NT-CR and the MD simulations for carbon, we successfully calculated the special distributions of the H and H_2, which gave agreement with the experimental measurement. We also found that a small amount of H_2 in the high rotational state is generated from the divertor plate. These H_2 molecules in the high rotational state are dissociated quite frequently by interacting with the electrons in the divertor plasma.
- Moreover, expanding the MD simulation to the isotopic hydrogen molecules which are desorbed from the divertor carbon plate, we obtained the population of the isotope hydrogen molecules for each rovibrational level.
- Finally, we calculated the desorption rate of H and H_2 from the tungsten crystal by the MD codes.

Combining NT-CR code, MD, and EMC3-EIRENE

Figure 13 from Y. Hayashi et al 2016 Nucl. Fusion 56 126006
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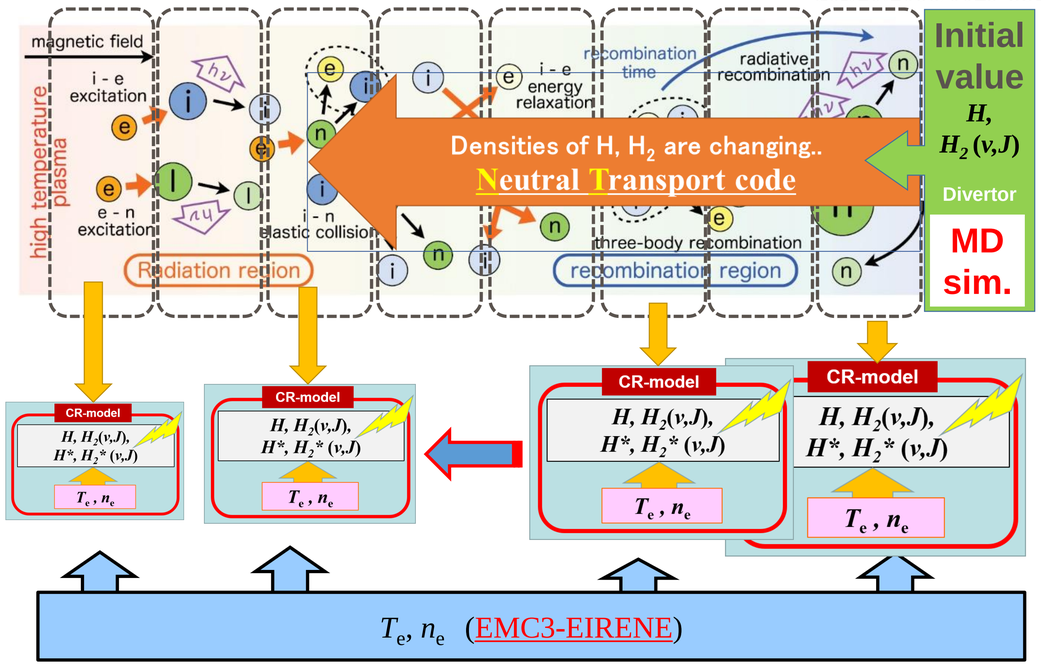
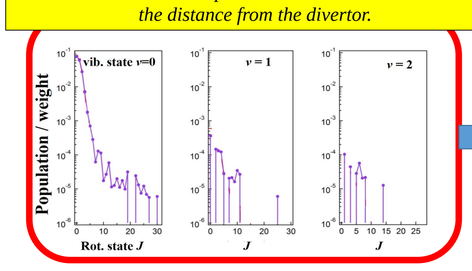
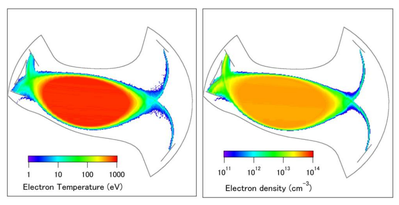


By NT-CR code, EMC3-EIRENE, MD, H_2 and H densities for LHD

Simulation results of the rotational level J dependence of population for three vibrational states (v=0,1, 2). The divertor material is amorphous carbon. Each color indicates the distance from the divertor.

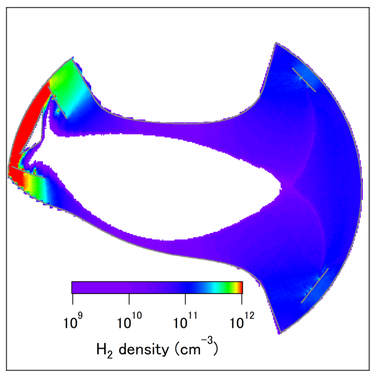


T_e & n_e by EMC3-EIRIRE



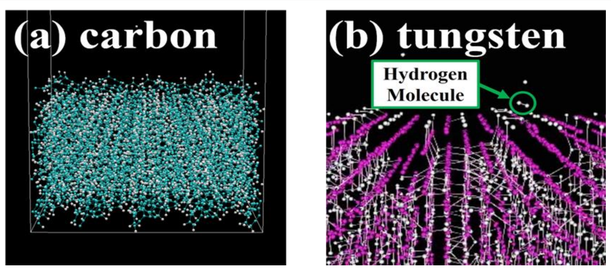
Neutral Transport code with CR model

The 3-dimentional spatial distribution of H_2 in LHD by the combining three codes, i.e., (1)NT-CR code, (2)EMC3-EIRENE code and (3)MD code for carbon in our previous work[3]. In the present paper, we focus on the divertor plasma region not only for carbon but also tungsten as divertor plate material.



MD simulation to calculate H and H_2 rovibrational population emitted from the divertor plate (graphite or tungsten).

The target in the MD simulation for divertor plate material. H atoms are distributed in amorphous carbon (a) and in tungsten bcc crystal (b), respectively. Blue, purple and white balls denote carbon, tungsten and hydrogen atoms, respectively.



Temperature of Target : 300K
Total Simulation Time : 50 ps
Incident Hydrogen : 1 atom & 50 eV
Incident angle: Parallel to z-axis
Boundary condition:
Periodic in x- and y- direction
Trial number: 1500
Δt = 0.01 fs

(a) CarbonAmorphous Carbon
* 3872 C atoms
* 2080 H atoms
- Interatomic interaction: Brenner's Potential

(b) Tungsten
* 4608 W atoms
* Sample TA: 2272 H atoms.
* Sample TB: 4368 H atoms.
* Sample TC: 6300 H atoms.
- interatomic interaction: EAM potential by Wang

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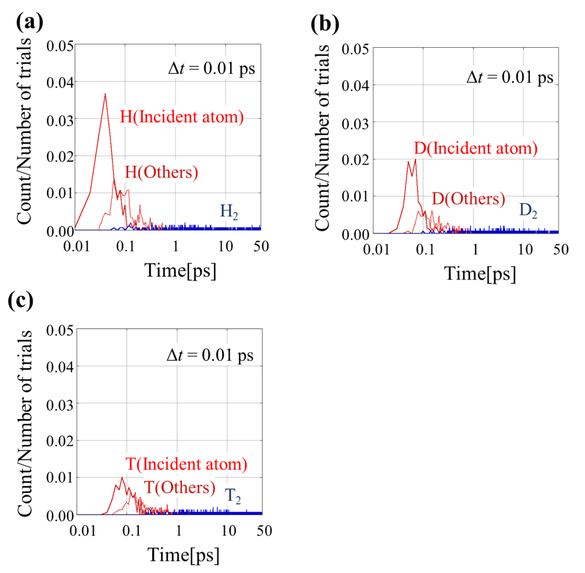
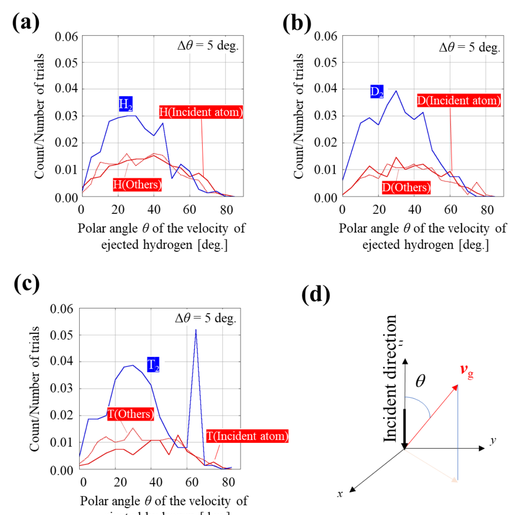
SIMULATION RESULTS (BY MD SIMULATION)

1. GRAPHITE:ISOTOPE Effect, D_2, T_2 Population with Rovibrational State (v, J)

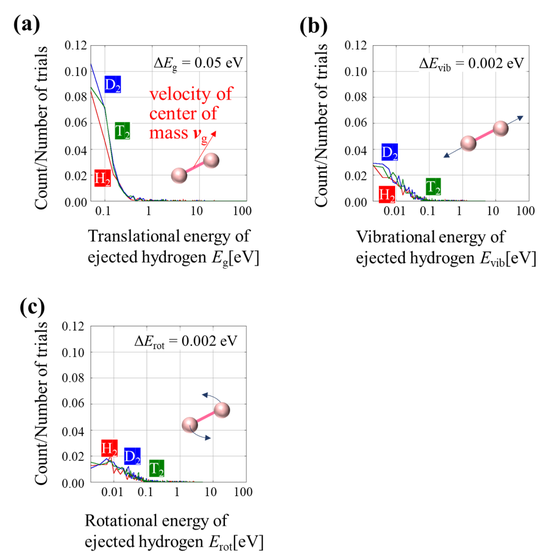
Emission time of emitted H, D, T atoms and H_2, D_2, T_2 molecules in (a), (b) and (c), respectively.



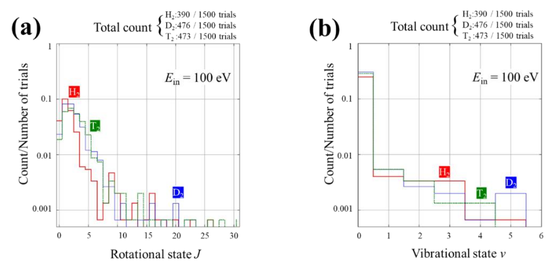
Emission angle distribution of emitted H, D, T atoms and H_2, D_2, T_2 molecules in (a), (b) and (c), respectively. The polar angle θ is defined in Fig. (d).



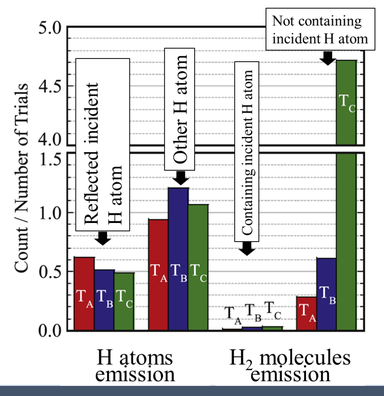
Distribution of translational (a), vibrational (b) and rotational (c) energy of emitted H, D, T atoms and H_2, D_2, T_2 molecules.



Distribution of rotational state J (a) and vibrational state v (b) of emitted H_2, D_2, T_2 molecules.



2. TUNGSTEN



Number of emitted hydrogen atoms and molecules in 1500 trials in three cases of tungsten targets (T_A, T_B, and T_C). The number of hydrogen atoms in each tungsten target is 2272, 4368, and 6320 for T_A, T_B, or T_C, respectively. The number of tungsten atoms is set to 4608 for all tungsten targets[8].

CONCLUSION

1. **Rovibrationally resolved neutral transport code for the molecular hydrogen is constructed.**
2. **The initial rovibrational state of the molecules released from the divertor wall is calculated by MD simulation.**
3. **The rovibrationally resolved neutral-transport code can be used for**
   a. **Evaluation of various effective reaction rate coefficients including MAR**
   b. **Analysis of observed emission spectra of hydrogen molecule.**
   c. **Evaluation of energy loss rate of the electron by the rovibrational excitation**
4. **We developed MD simulation for hydrogen recycling on carbon divertor for H, D, and T.**
5. **We calculated distributions of emission angle, translational, vibrational and rotational energy of emitted atoms and molecules for H_2, D_2, and T_2.**
6. **We calculated the desorption rate of H and H_2 from the tungsten crystal by the MD codes.**

ACKNOWLEDGEMENTS / REFERENCES

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