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Tungsten sputtering by simultaneous deuterium and nitrogen

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Background

- **Fusion reactor** Reduction of heat load by impurity
  Seeding impurity gas nitrogen is considered to reduce the local heat load on the divertor by radiative cooling.
- **D+N simultaneously irradiation**
  N for cooling and deuterium (D) as fuel simultaneously collide with tungsten (W)
  Complex composition of N, W, D at surface due to sputtering.
- **W impurity in core plasma** Plasma temperature decreases by W impurity
  Sputtered W by N flows into the core plasma
  →plasma temperature decreases due to radiation loss.

It is important to understand W sputtering with simultaneous D+N irradiation.

Purpose

- Investigate W sputtering yield focused on the effect of irradiation energy and surface composition change by temperature.
  - ➢ Simultaneous irradiation of D + N → W is performed.

Summary

Comparison between experiment and simulation

- Experimental and TRIDYN simulation considering only physical sputtering are consistent within the range of about 30 %.
- E_N ≥ 500 eV, temperature dependence was not observed. At 700 K, 20 % higher yield than other temperature.
- E_N ≤ 350 eV, temperature dependence is visible. There is a possibility of difference in N surface concentration or the influence of other sputtering.

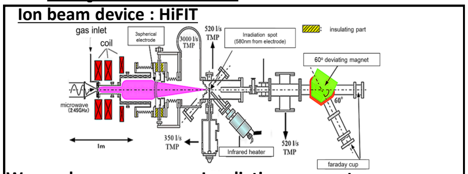
From simulations

- By changing energy ratio of nitrogen and deuterium (E_N/E_D) between 1.0 and 2.0 results in about 2 times the W sputtering yield.
- The influence of surface N concentration increases with irradiation energy increasing (up to 40%).

Experiment and Simulation

Experiment

Ion beam device : HiFIT



W sample
- ➢ Size : 10 × 10 × 1[t] mm
- ➢ Single side mirror polished
- ➢ 1273 K 1h anneal
- ➢ Sputtering yield is calculated from mass loss.

Irradiation parameter
- ➢ V_{ACC} (Acceleration voltage) : 0.3 ~ 1.0 kV
- ➢ D+N fluence: 1.0 × 10^{24} /m^2
- ➢ Sample temperature : 400 ~ 700 K
- ➢ N concentration: 3.5 %
- ➢ Irradiation area: Φ5 mm

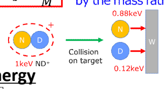
Ion species and ratio in the HiFIT ion beam

Ion species	D^+	D_2^+	D_3^+	N^+	ND^+	ND_2^+	ND_3^+	ND_4^+
Ratio [%]	38.4	17.4	36.5	0.3	1.1	1.6	3.5	1.3

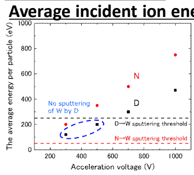
$$E_{atom}[\mathrm{eV}] = E_{molecule}[\mathrm{eV}] \times \frac{m}{M}$$

Distributed by the mass ratio

- E_{atom} :Energy of atom in molecule
- $E_{molecule}$:Energy of molecule
- m :Mass of atom
- M :Mass of molecule



Average incident ion energy

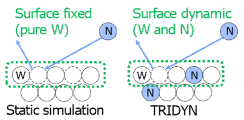


- ➢ E_N is higher E_D and its ratio E_N / E_D is about 1.6.
- ➢ The average energy of D (E_D) is about 50% of $V_{ACC.}$
- ➢ The average energy of N (E_N) is about 75% of $V_{ACC.}$

Simulation

TRIDYN Simulation

Dynamic binary collision approximation code[1].
Can consider changes in surface composition.



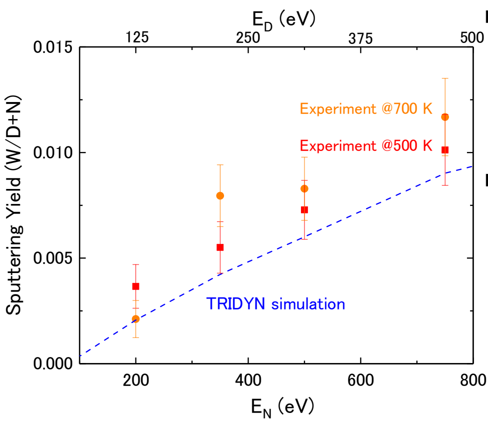
Parameters	Setting
Target	Tungsten
Irradiation energy	D 120~470 [eV]
	N 200~750[eV]
Fuluence	1 × 10^{24} [/m^2]
D : N	96.5 : 3.5 [%]
D-D Surface Binding Energy (S.B.E.)	0 [eV]
D-N S.B.E.	0 [eV]
D-W S.B.E.	0 [eV]
N-N S.B.E.	9.79 [eV] [2]
N-W S.B.E.	6.7 [eV] [3]
W-W S.B.E.	8.79 [eV] [4]

[1]Wolfhard Moller and Wolfgang Eckstein, Binary collision Simulation of Atomic Collisions Dynamic Composition Changes in Solids, IPP 9/64 (1988)
[2]NN Misra, Oliver Schlüter, PJ Cullen Cold Plasma in Food and Agriculture: Fundamentals and Applications (2016)
[3] Harold F. Winters and Peter Sigmund," Sputtering of chemisorbed gas (nitrogen on tungsten) by low - energy ions" Journal of Applied Physics 45, 4760 (1974);
[4] CRC Handbook of Chemistry and Physics, 78th ed., 11-42ff

Results

Experiment and Simulation

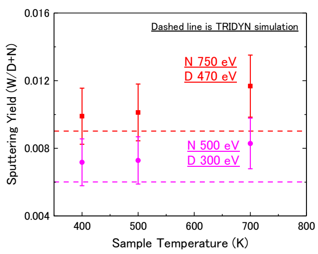
Incident ion energy dependence



Comparison between 500 K experiment and simulation
- ➢ The error is around 20 % between experimental and simulation.
  It is considered that the influence of physical sputtering is very high.

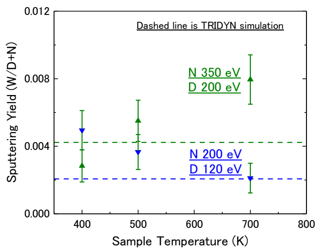
Comparison between 700 K experiment and simulation
- ➢ Sputtering yield is higher than 500 K.
  Some values are out of error bars.
- ➢ The error is around 30 % between experimental and simulation.
  It is out of the error bar,
  but the influence of physical sputtering is still large.

Sample temperature dependence



E_N ≥ 500 eV
Temperature dependence was not observed.
➢But at 700 K, 20 % higher yield.

Since physical W sputtering yield changes due to surface N concentration.
There is a possibility of N desorption from W surface at 700 K.



E_N ≤ 350 eV
Temperature dependence was observed.
- ➢ The experimental data is not consistent with the simulation.
- There is a possibility that such temperature dependence arises due to change in N surface concentration.

→Surface composition analysis is planned. (by XPS)

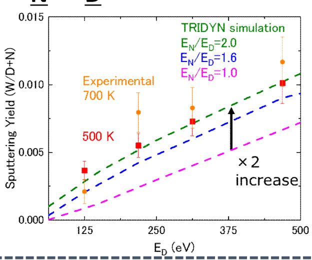
Simulation of physical sputtering

Compared to experimental result, TRIDYN simulation was about 20 to 30% lower.

Possible reasons :
- ➢ E_N/E_D=1.6 energy distribution was not accurate.
- ➢ N desorption from the surface due to temperature effects may lead to lower N surface composition.

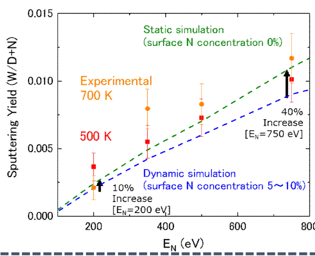
Clarify two points by simulation.

E_N/E_D dependence



- E_N/E_D was changed within the range of 1.0 to 2.0.
- ➢ E_N/E_D =2.0, simulation fits experimental data better.
  - When the beam strikes the sample, E_N may be larger than the assumed value.
- ➢ E_N/E_D was varied from 1.0 to 2.0.
  - The changes in the energy ratio (E_N/E_D) results in W sputtering to vary by a factor of two.

Effect of N concentration on W surface



- Compared N surface composition static and dynamic by performing TRIDYN simulation.
- ➢ Static case: sputtering yield increased by 10 to 40%.
  - As the irradiation energy increases, the difference increases.
- ➢Static simulation fits the experimental data better.
  Sample temperature may be affected.

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