Dynamic Simulation of Erosion and Redeposition on Plasma Facing Materials

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With contribution from

[*1] A. Sagara and LHD Experimental Group; [*2] V. Philipps , T. Tanabe and TEXTOR team; [*3] T. Tanabe

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Dynamic Monte Carlo simulation code, *EDDY*

- **Plasma ion irradiation on solid surfaces**

  (1) Simultaneous bombardment with hydrogen and impurity ions ;

  $D^+ + C^{4+}, Be^{2+}, O^{4+}, Fe^{4+}, W^{4+}$

  (2) Maxwellian velocity distribution and sheath acceleration

  ; $T_e = T_i$ and $V_{sh} = -(T_e/2)\ln(\pi m_e/m_i)$

- **Dynamic erosion and deposition processes**

  (3) Physical sputtering and plasma impurities deposition

  (4) Chemical erosion due to hydrocarbons formation

  (5) Collisional mixing and thermal diffusion

  ;10^7~10^8 pseudo-ions for 10^{25}~10^{26} m^{-2}; 400 surface layers in Δx=20 nm;

  ; atomic density $n_{W\text{-}C}$ is $(n_{W\text{-}C})^{-1} = f_W(n_W)^{-1} + f_C(n_C)^{-1}$, where $f_W + f_C = 1$.

- **Impurity transport in near-surface plasma**

  (6) Multiple ionizations and dissociations of sputtered and reflected impurities, including H and H_2, and CH_4 and higher hydrocarbons

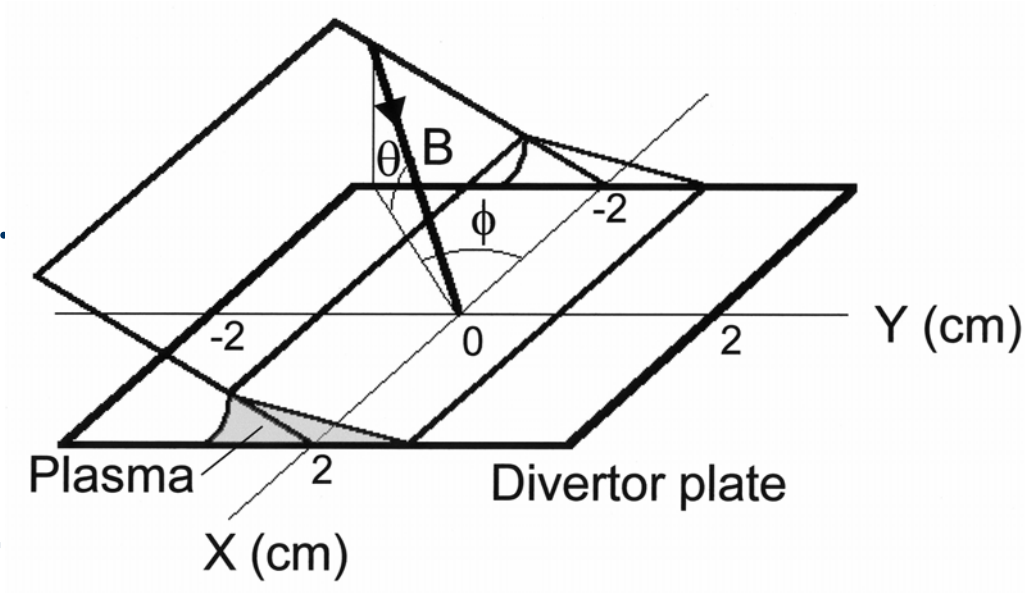
  (C_2H_2, C_2H_4, C_2H_6, C_3H_6)

  (7) Gyromotion of the ionized impurities, simultaneously receiving collisional friction force

Erosion/deposition patterns and impurity depth profile of a LHD divertor tile

- The erosion and redeposition patterns and depth profile of the deposited impurities provide us important information regarding the local transport.

- The *EDDY* code is applied in order to simulate the erosion and redeposition patterns on a graphite plate which was used in the 3rd experimental campaign of the large herical device (LHD).

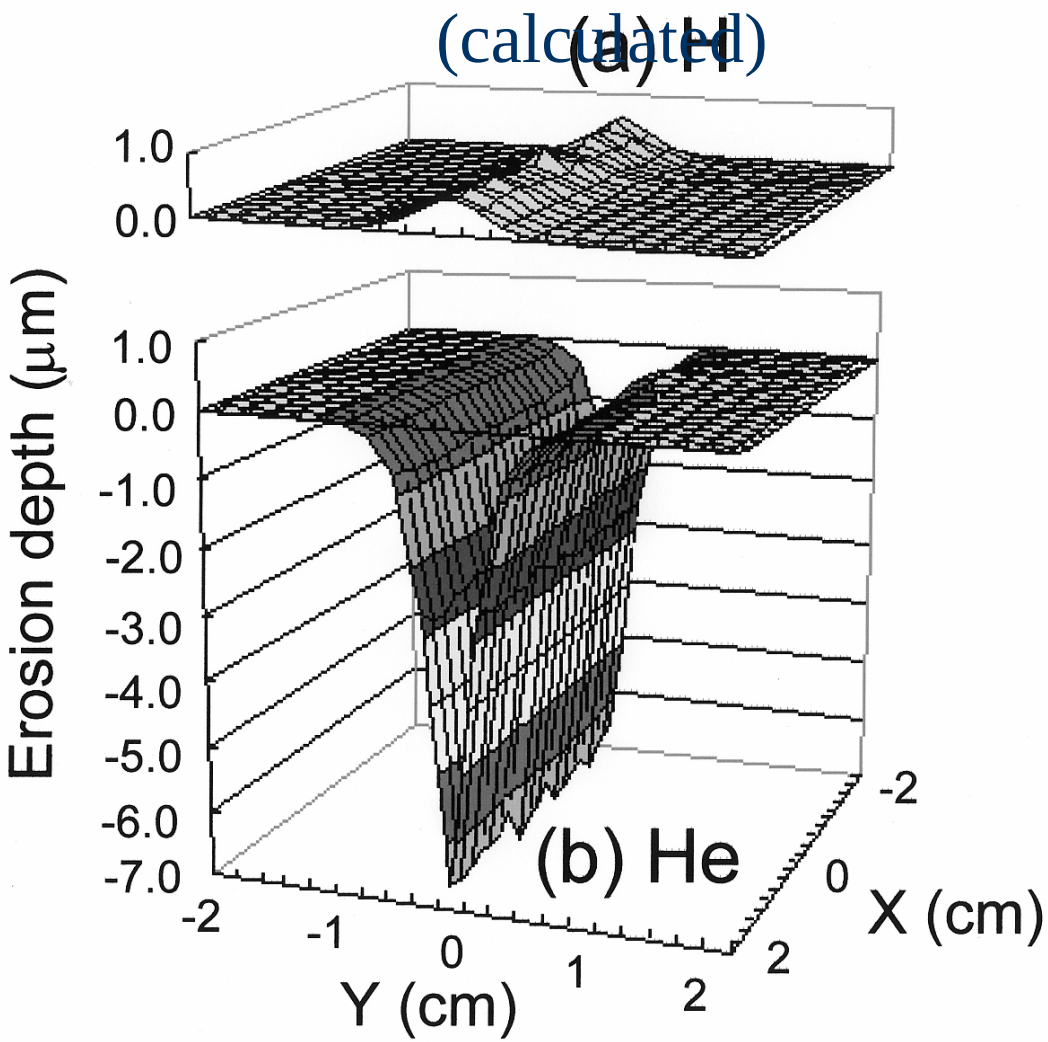


$n_{e0}=10^{12}$ cm^{-3}, $\lambda_n=0.55$ cm
$T_{e0}=T_{i0}=24$ eV, $\lambda_T=0.55$ cm
B=1 T; θ=39.4 deg, ϕ=46.9 deg
Ion fluence: 2×10^{21} cm^{-2} (He plasma)
1×10^{21} cm^{-2} (H plasma)
Impurities: C^{4+}(2%), O^{4+}(1%), Fe^{4+}(0.1%)
Initial Fe deposition on C: 0.0035 μm

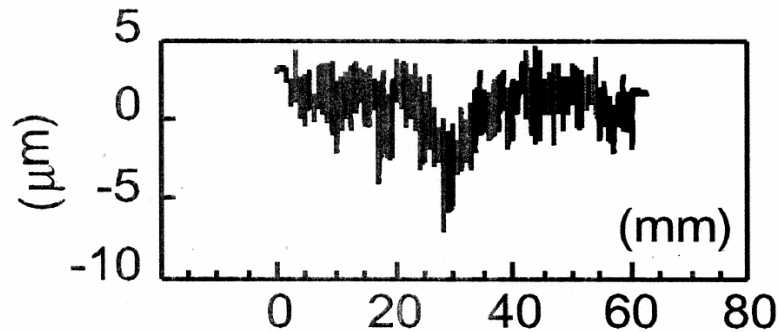
Simple divertor geometry used for calculation

An area on the plate is divided into many segments: $N_X \times N_Y \times N_{depth}$

- Erosion and redeposition patterns (calculated)



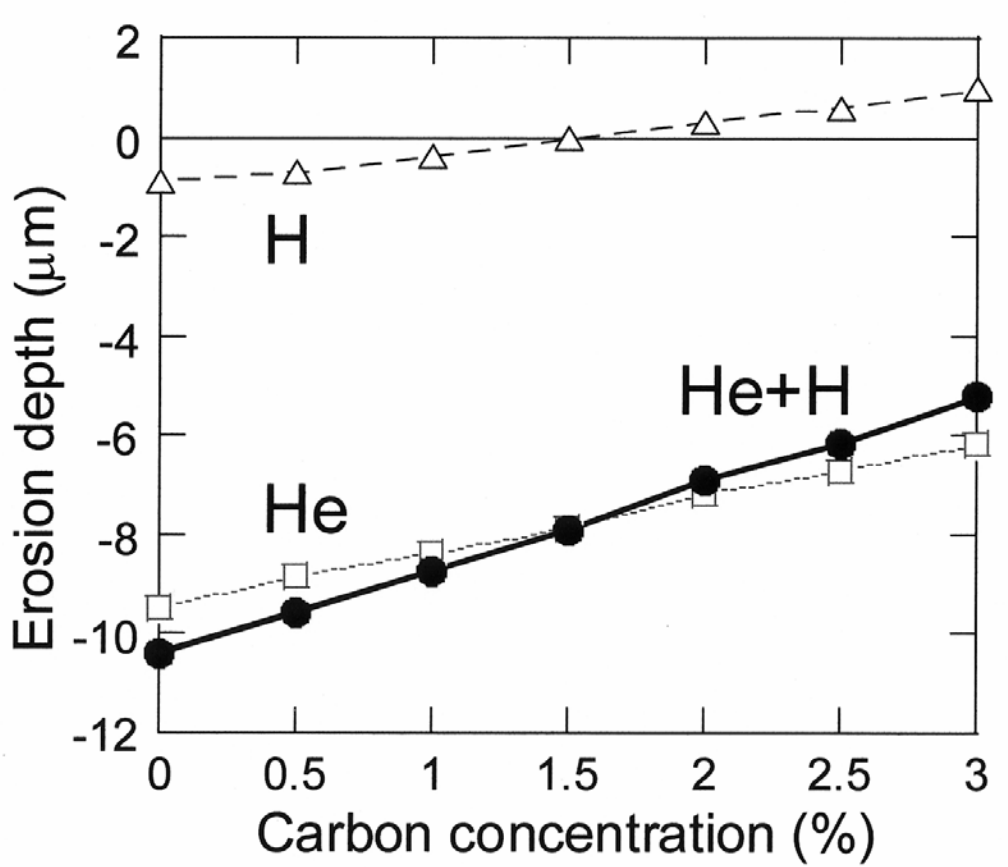
- LHD graphite divertor tile (measured)



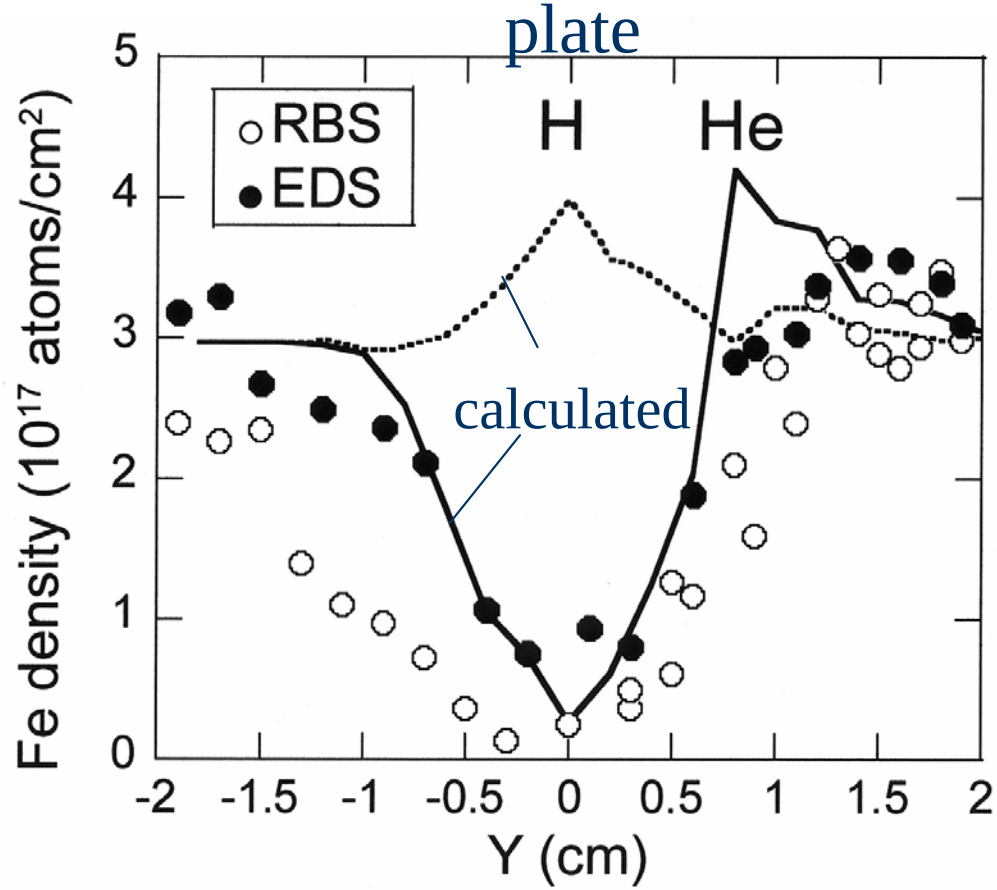
Measured
(Sagara et al., PSI15)

- The He plasma causes net erosion, but the H plasma causes net deposition.
- The total net erosion is close to the measured depth (~6μm).

■ Erosion depth as a function of carbon concentration of H and He plasmas

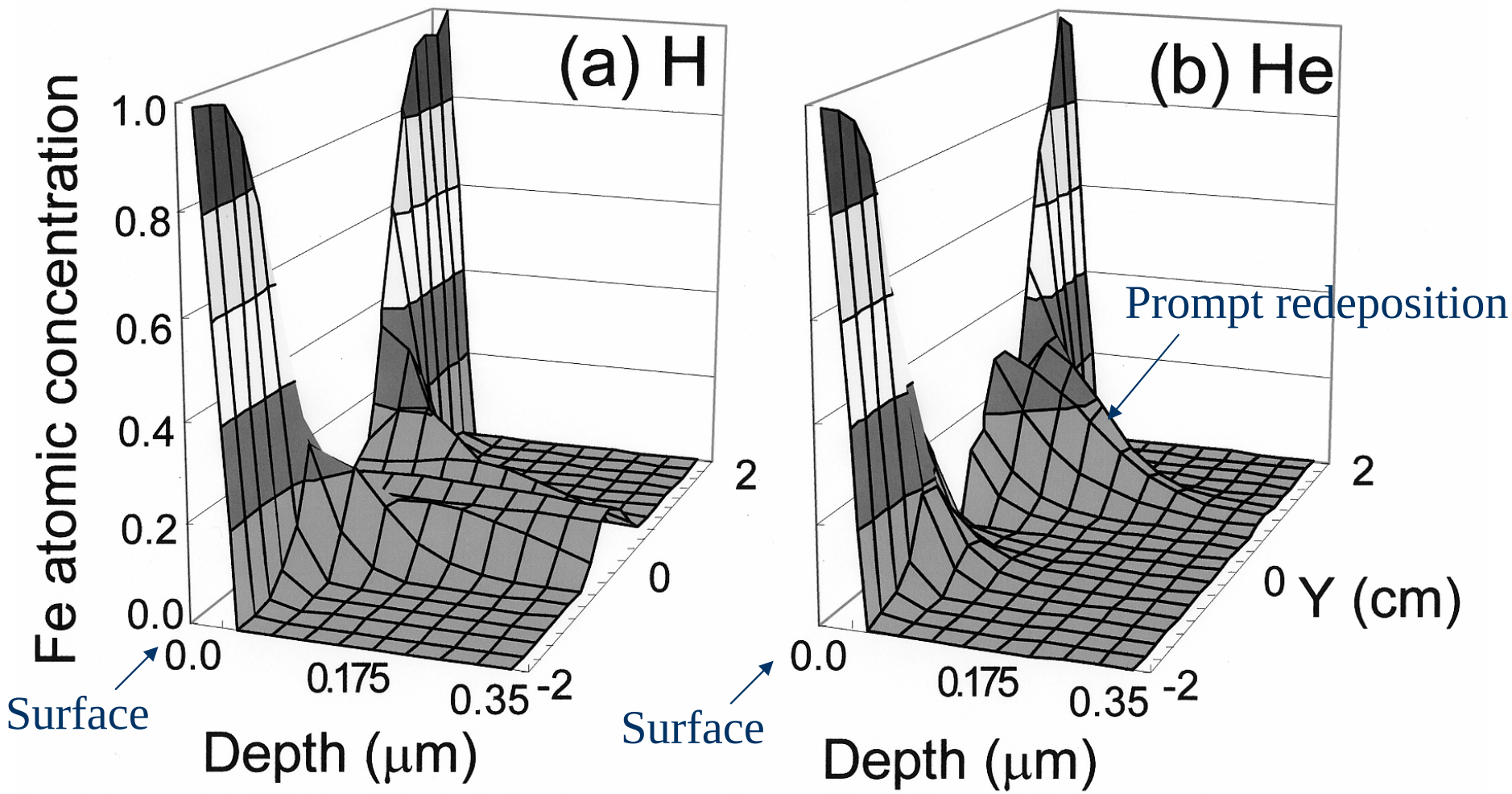


■ Calculated and observed Fe distributions on the divertor plate



- The erosion and deposition are influenced by the concentration of impurities.
- The distribution of Fe atoms integrated throughout the entire depth reproduces the observed Fe densities, which is dominated by the He discharges.

■ Depth profiles of Fe atoms after exposures of (a) H plasma and (b) He plasma

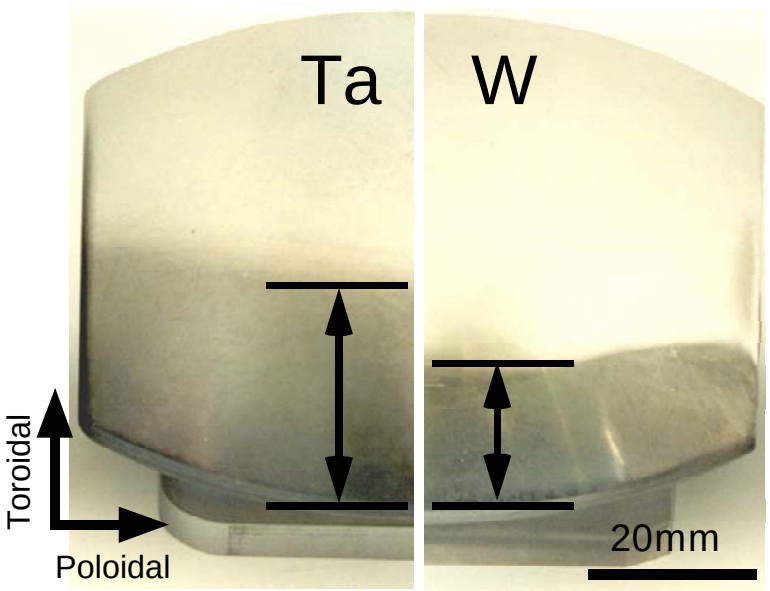


- For H plasma, C deposition reduces Fe atom density at the top layer of the surface, and Fe atoms are distributed inside the bulk.
- For He plasma, Fe atoms are strongly sputtered at the early stage of exposure, and prompt redeposition produces an asymmetric depth profile.

Erosion/deposition on W and C exposed to plasmas containing C and Be impurities

- After the plasma exposure in TEXTOR, erosion area and deposition area of the W-Ta twin test limiter are clearly separated each other.

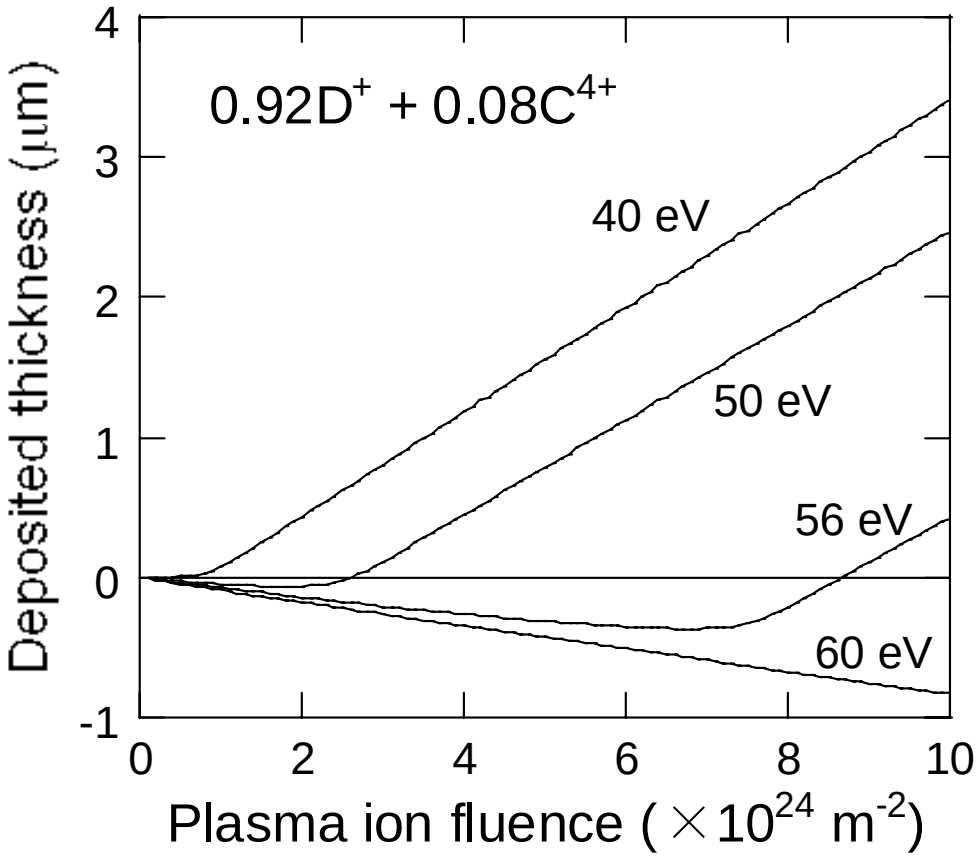
- The extent of the deposition area was distinctly broader on Ta than on W exposed to the plasma under the same condition.

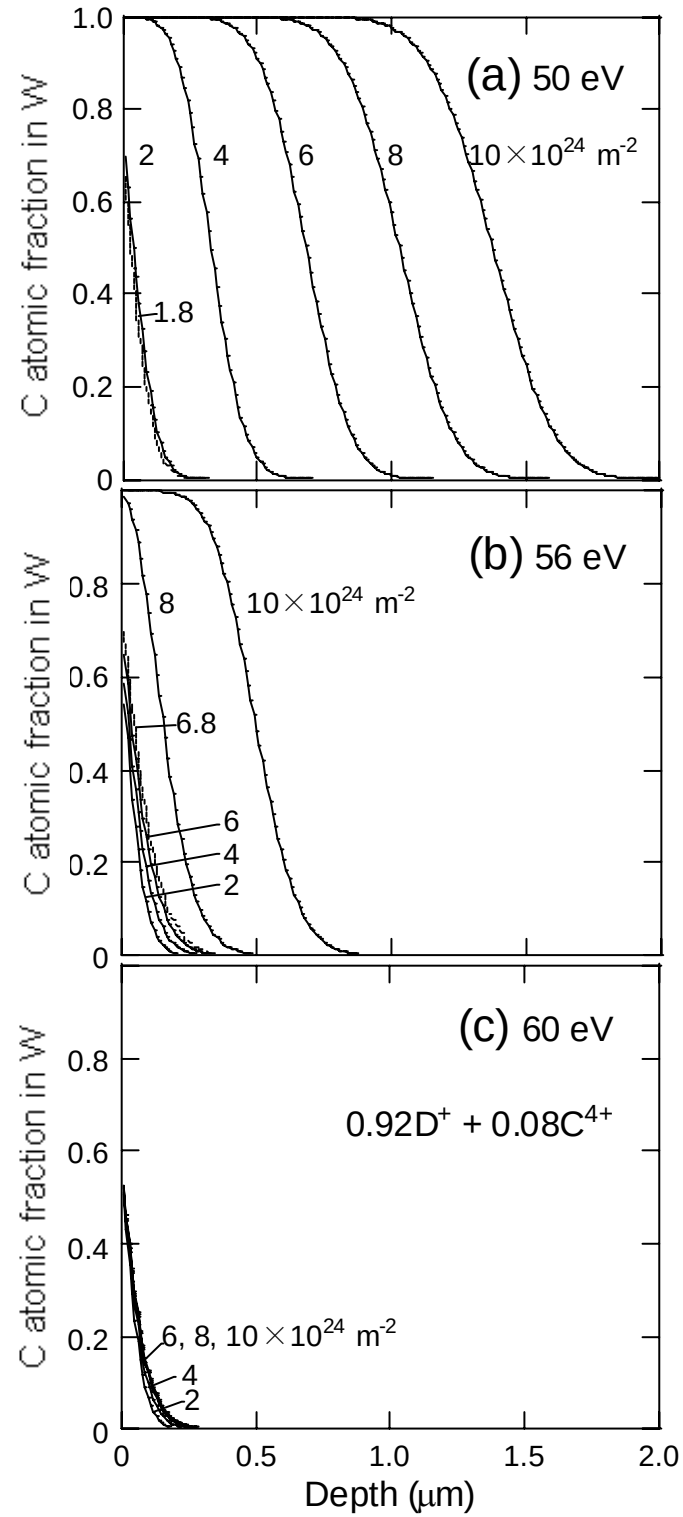


View of C deposits on the Ta and W parts of the W-Ta twin limiter in TEXTOR.(T.Hirai, et al., JNM)
Plasma ion flux : 10^{18} – 10^{19} $m^{-2}s^{-1}$
Total exposure time : 231 s (W)
136 s (Ta)

Transition behavior between erosion and deposition is investigated during high-fluence (10^{19} ~10^{22} cm^{-2}) plasma exposure, by using the *EDDY* code.

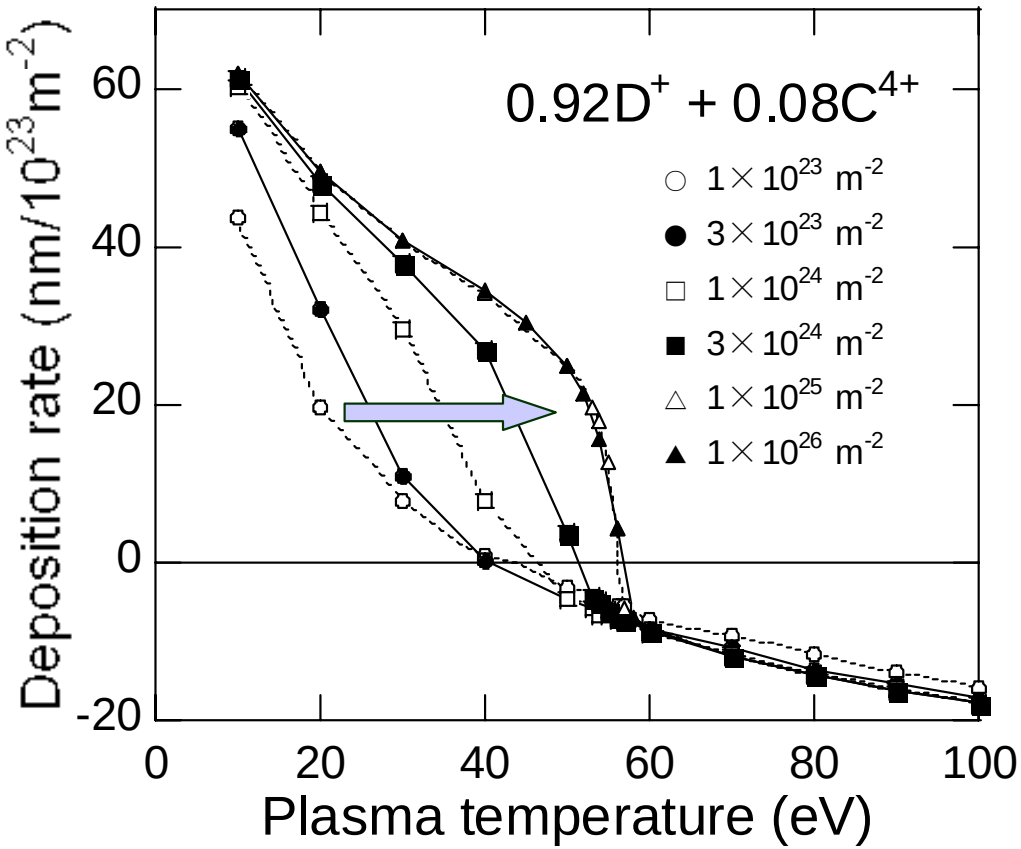
■ Plasma ion fluence dependence of erosion and deposition on W

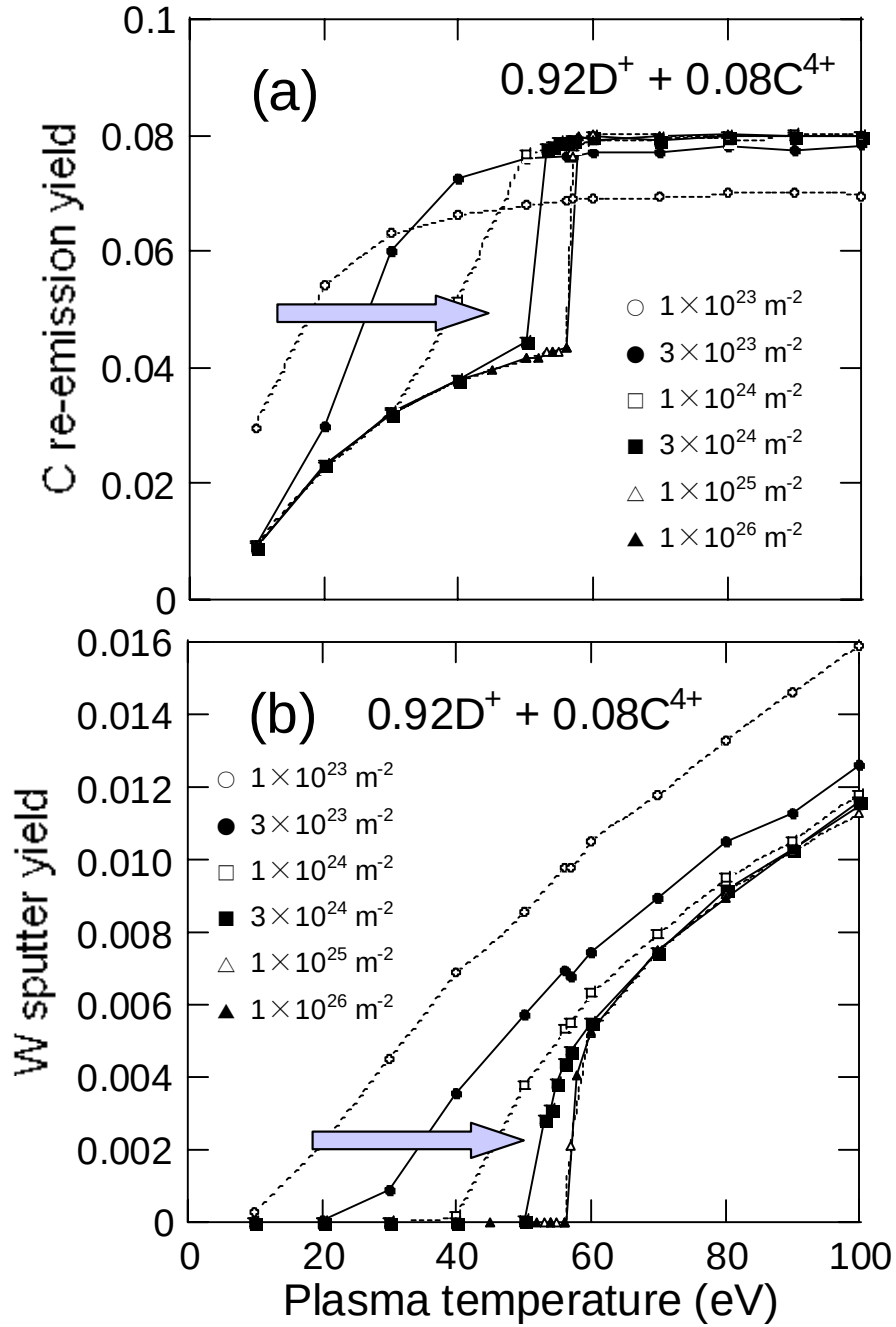




- At intermediate temperatures, the transition from erosion to deposition occurs during the exposure.
- At high temperature, the amounts of the deposited C and released C are balanced on a W-C mixed layer.

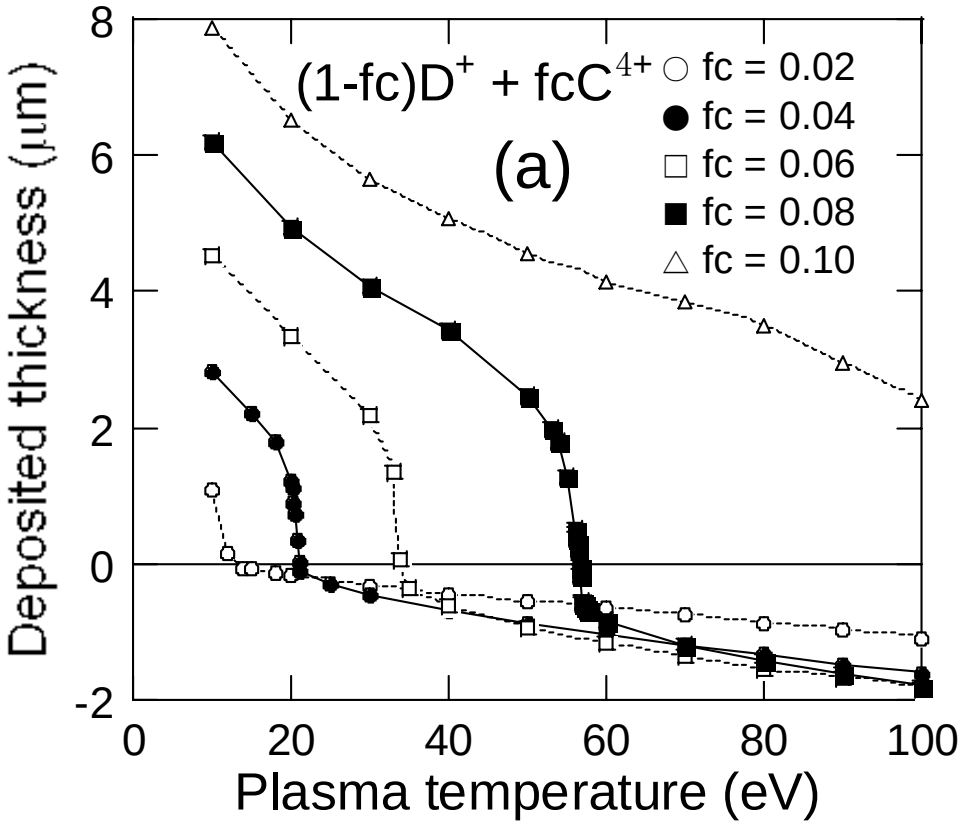
■ Plasma temperature dependence of erosion and deposition

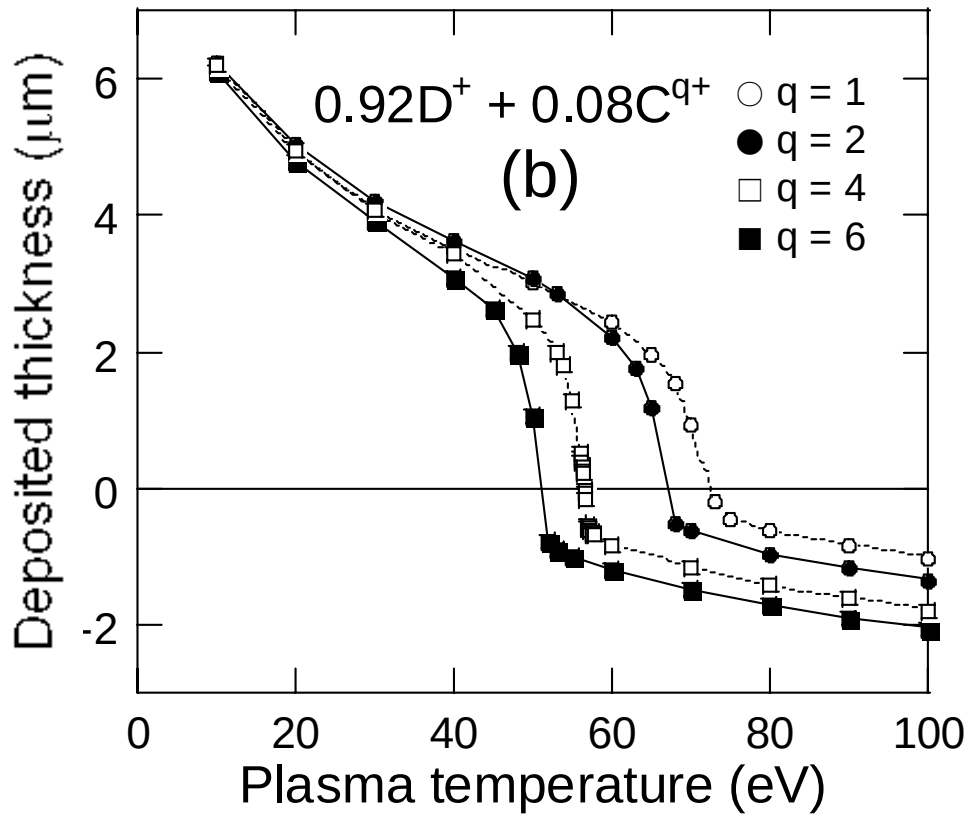




- Plasma temperature dependence of the deposition rate changes dynamically with increasing plasma fluence.
- Finally, a sharp transition is formed.
- The thick C layer causes the C re-emission yield to decrease at low temperature.
- At high temperature, the C and W yields approach fluence-independent values for a W-C layer.

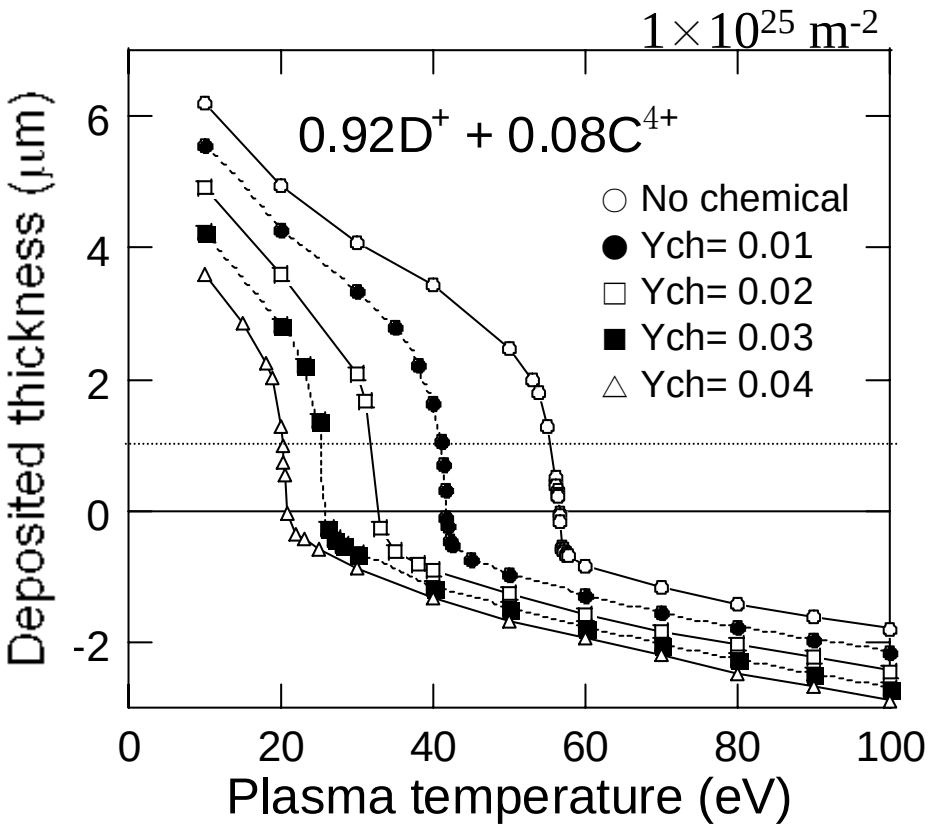
■ Changes of erosion and deposition with concentration and charge state of C ions in a plasma

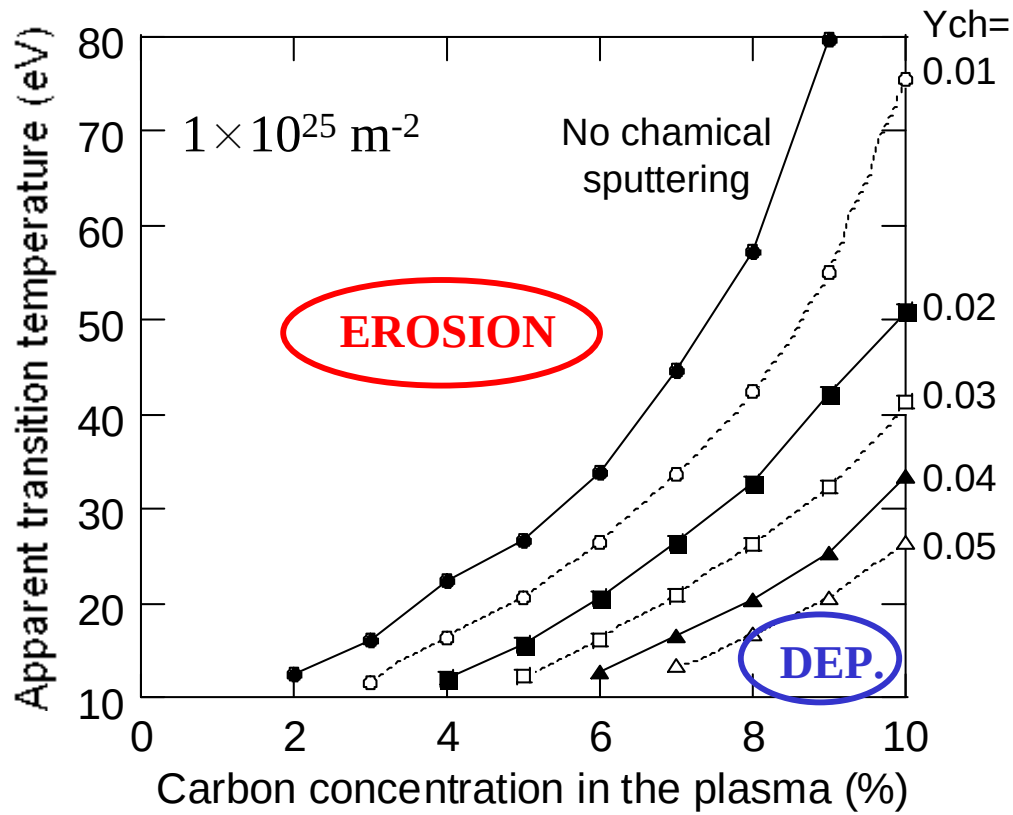




- The W-C mixed layer is eroded by the impact of a small amount of C ions (<10%).
- The thick C layer is mainly eroded by D ions (>90%).
- The transition temperature increases with increasing C concentration and decreasing charge state of C ions.

■ Change of erosion and deposition with chemical erosion



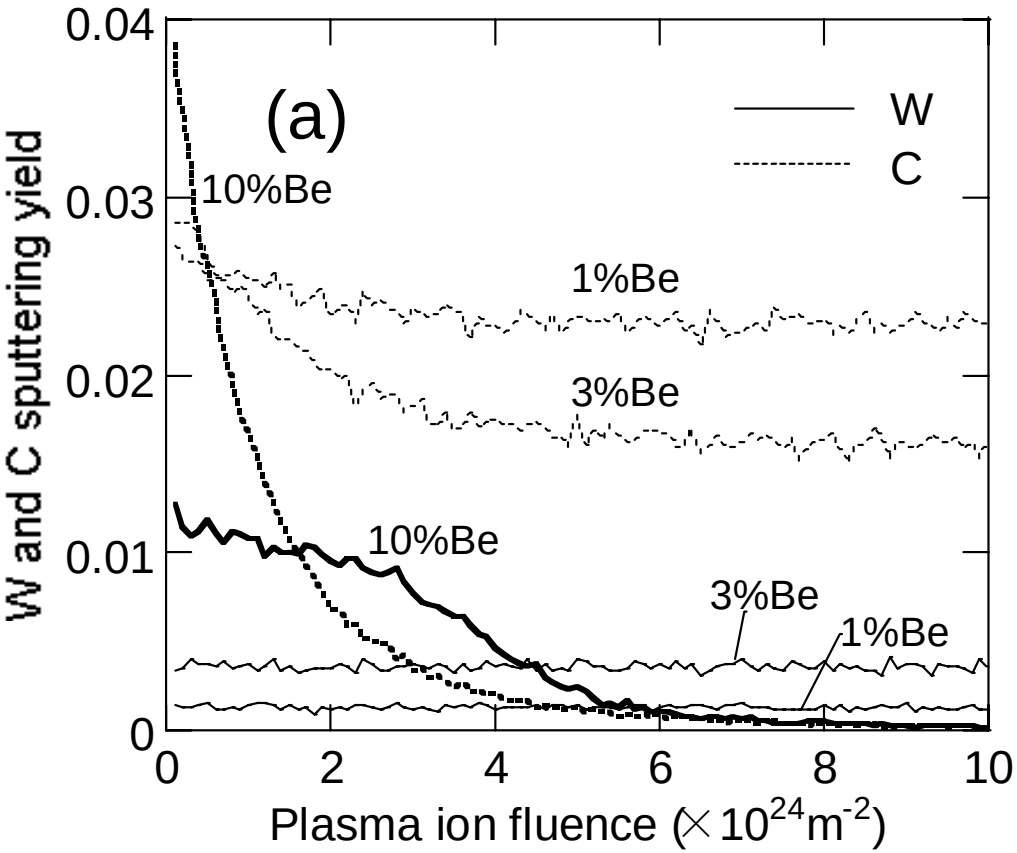


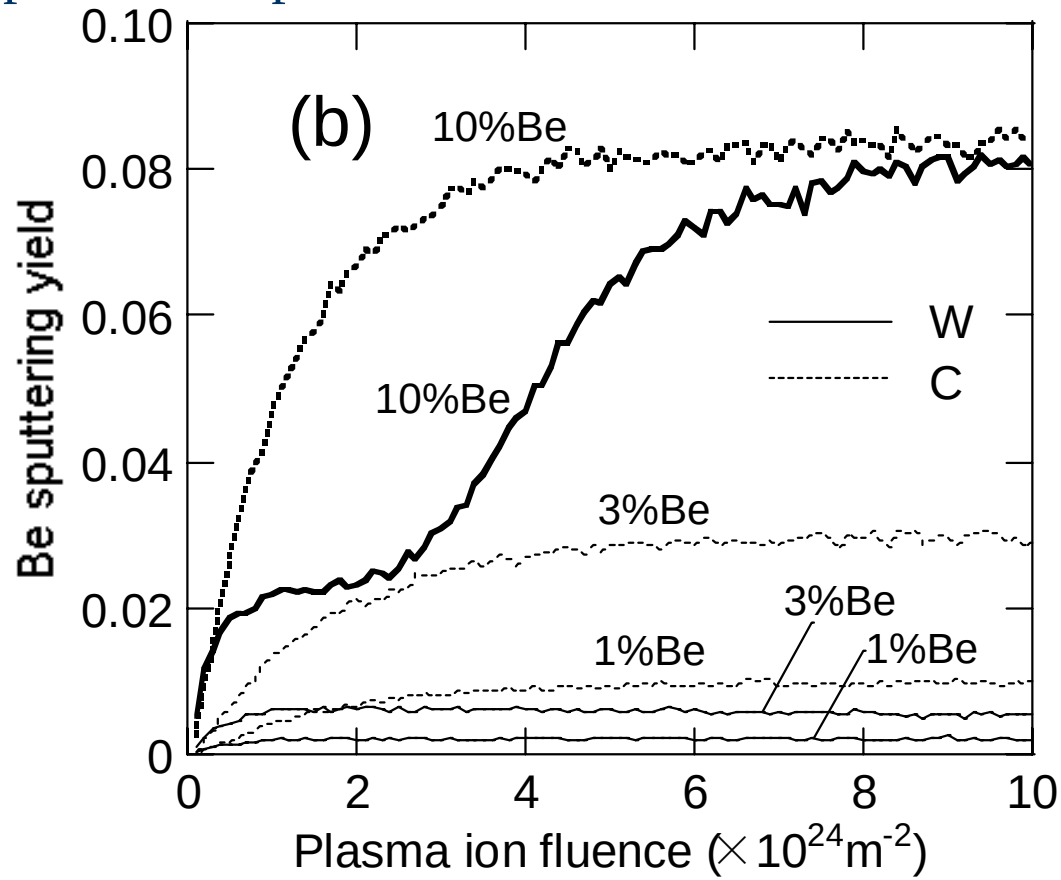
- Including chemical erosion, C depth profile in W is clearly localized at the surface and a steady state condition is reached at lower plasma temperature.

- "Apparent" transition temperature is defined as the temperature where the deposited thickness decreases to be 1μm at the ion fluence of 10^{25} m^{-2}.
- High C concentration and low plasma temperature enhance the C deposition on W.

■ Dependence of (a) W and C and (b) deposited Be sputtering yields on the plasma ion fluence as a function of the Be plasma concentration

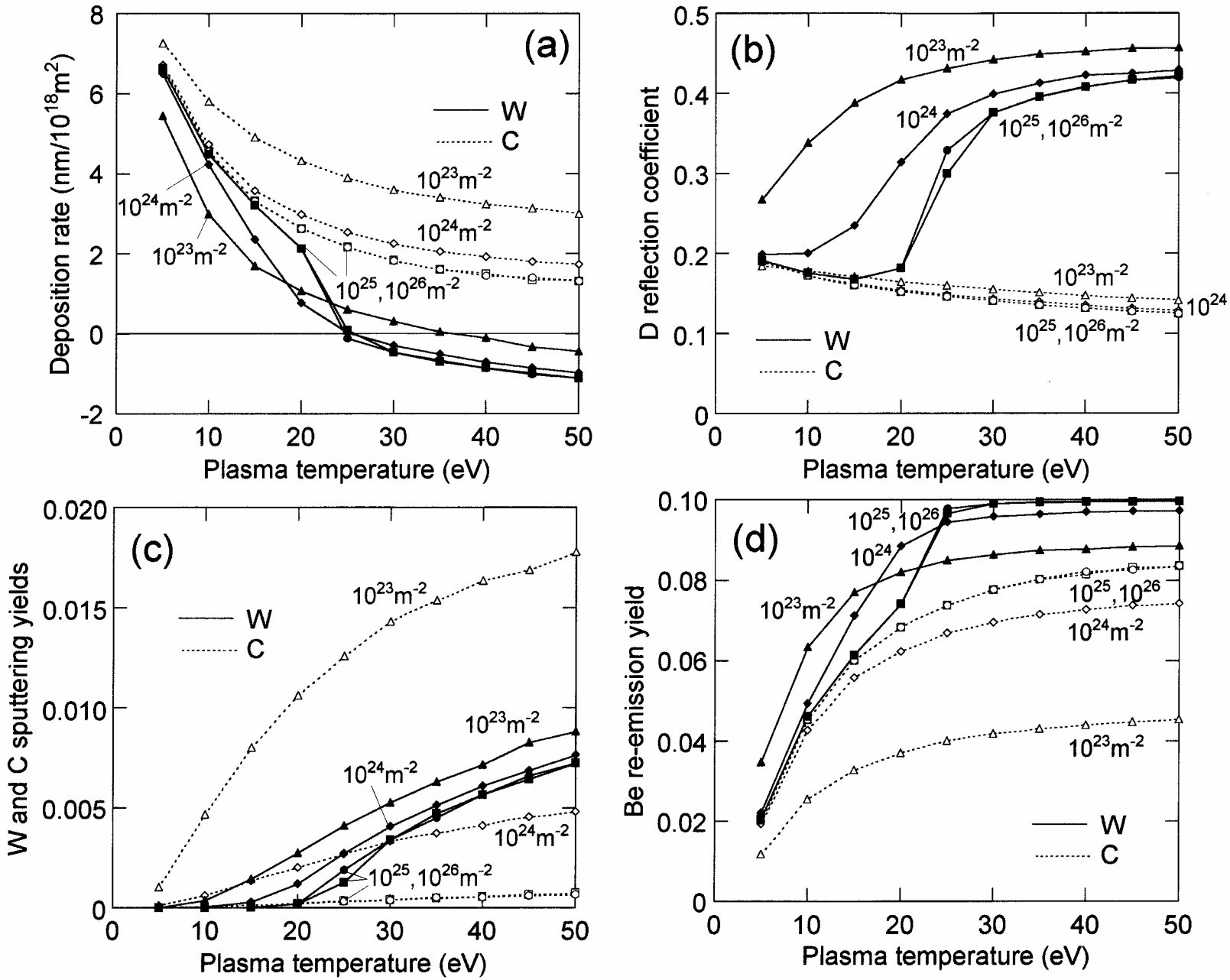
The plasma temperature is assumed to be 50 eV.





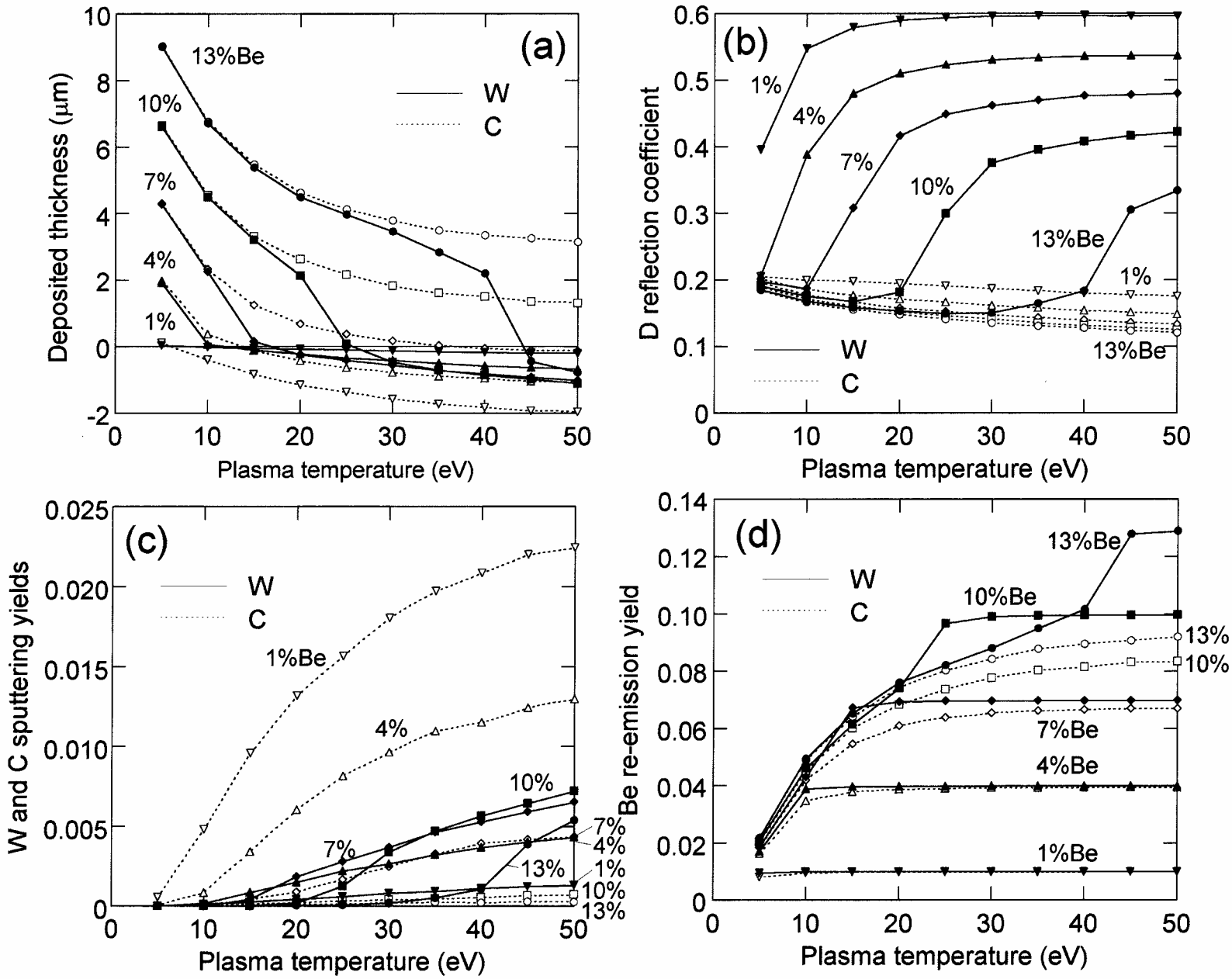
- There appears a step-like change in the sputtering yield of deposits (Be) on W during the exposure, however, a steady-state condition is reached at the fluence of 10^{25} m^{-2}.
- At low Be plasma concentration (<3%), the Be sputtering yield of C is approximately equal to the Be plasma concentration where the Be depth profile in C is unchanged during the plasma exposure.

■ Dependences of (a) deposition rate, (b) D reflection coefficient, (c) W and C sputtering yield and (d) Be re-emission yield on the plasma temperature, as a function of the plasma ion fluence



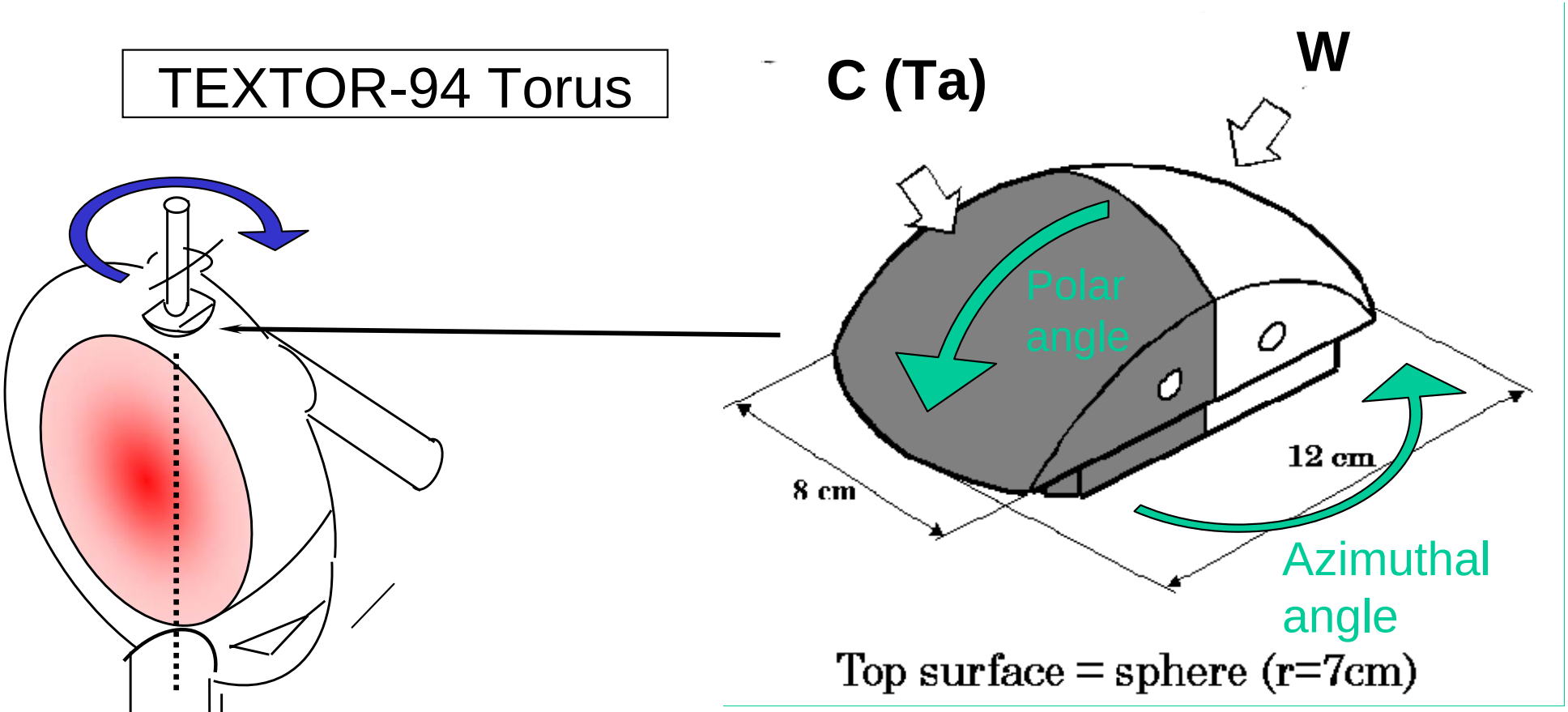
- The Be concentration is 10%.
- At high-fluence exposures (>10^{25} m^{-2}), a steady-state condition is reached.
- With increasing temperature, a transition from Be deposition to W erosion occurs similarly to the case of C deposition on W.

- Dependences of (a) deposition thickness, (b) D reflection coefficient, (c) W and C sputtering yield and (d) Be re-emission yield on the plasma temperature, as a function of the Be plasma concentration



- The total plasma fluence is 10^{25} m^{-2}.
- At the Be plasma concentration of less than ~4 %, a balance between the incident and released Be is reached for both C and W at the plasma temperature of more than ~10 eV due to the formation of Be-W and Be-C mixed layers.

■ W-C(Ta) twin test limiter experiments in TEXTOR



- A spherical surface of a W-C(Ta) twin test limiter in TEXTOR edge plasmas is devided into $N_{polar} \times N_{azimuth} \times N_{depth}$ segments.

  (N_{polar}=10, $N_{azimuth}$=36, N_{depth}=10)

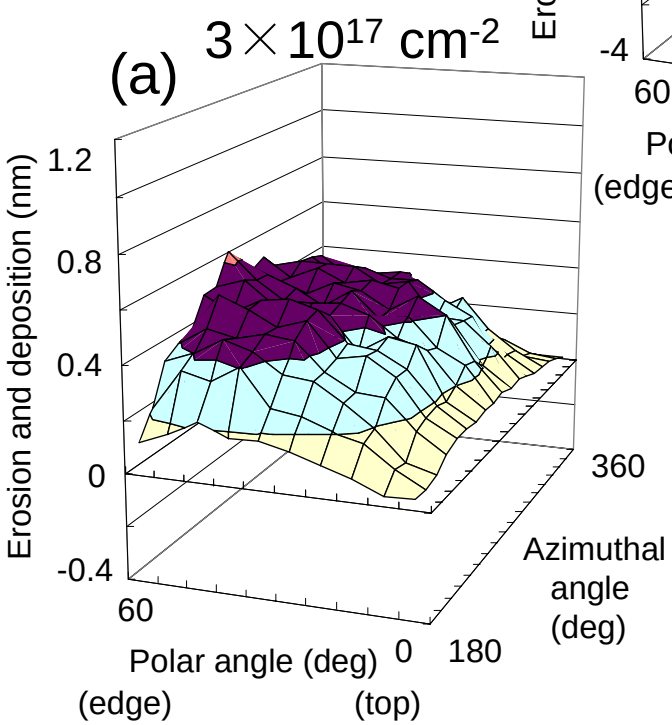
- TEXTOR edge plasma (at the top of the limiter)

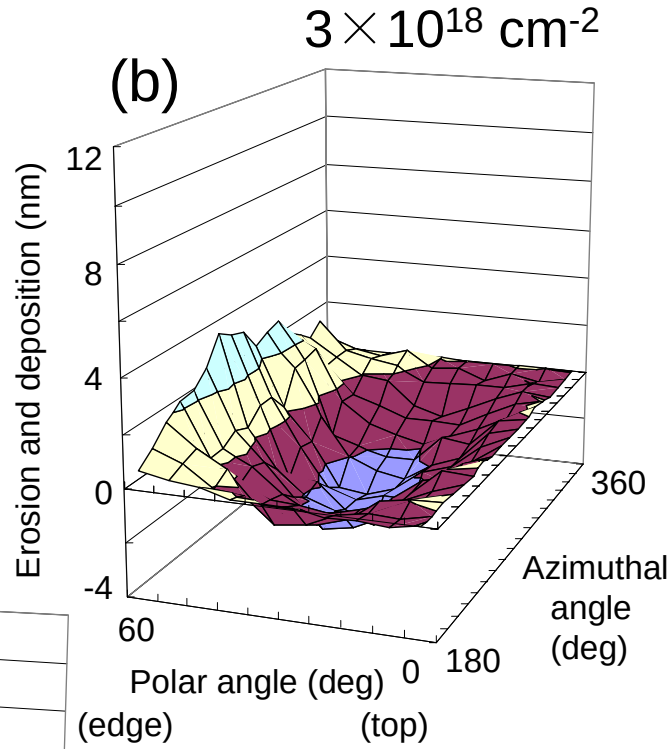
  n_e=5.2x10^{12} cm^{-3} (λ_{ne}=3.26 cm); T_e=64 eV (λ_{Te}=2.56 cm)

  B=2.25 T; D^+ : C^{4+} =98% : 2%; Te=Ti is assumed.

■ Erosion and deposition patterns on W side of W-C twin limiter

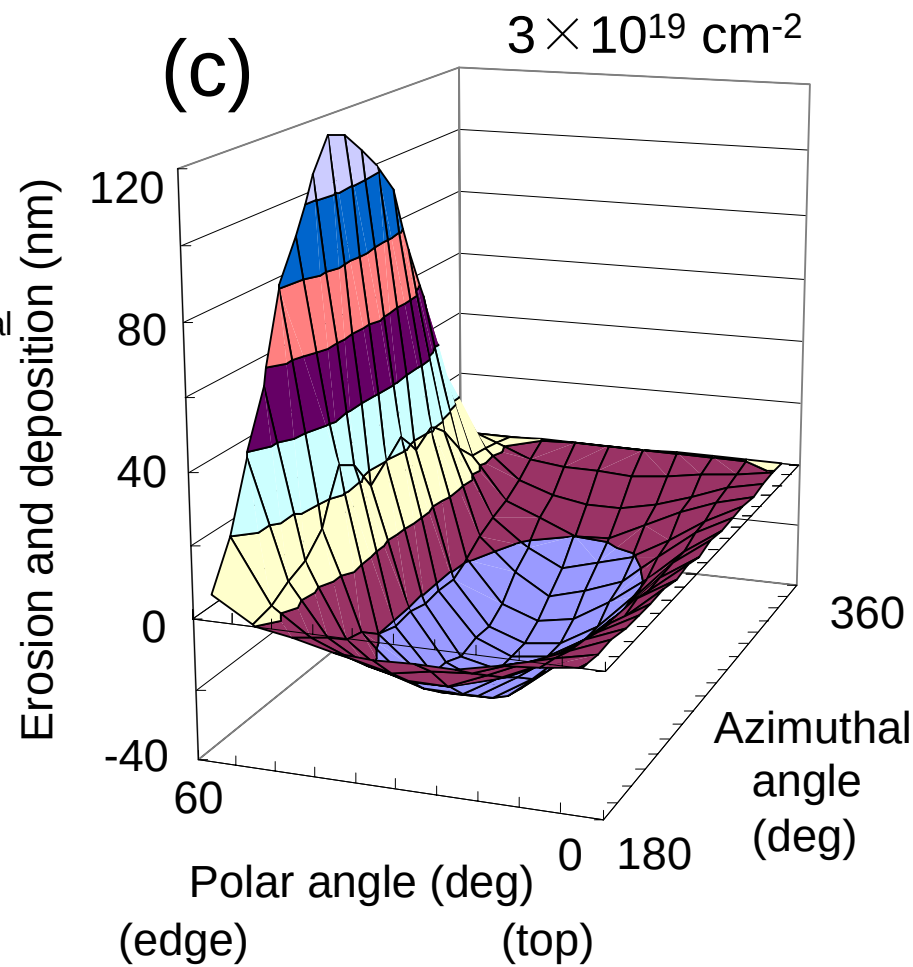
(a) At early stage of exposure, whole W side is covered by C



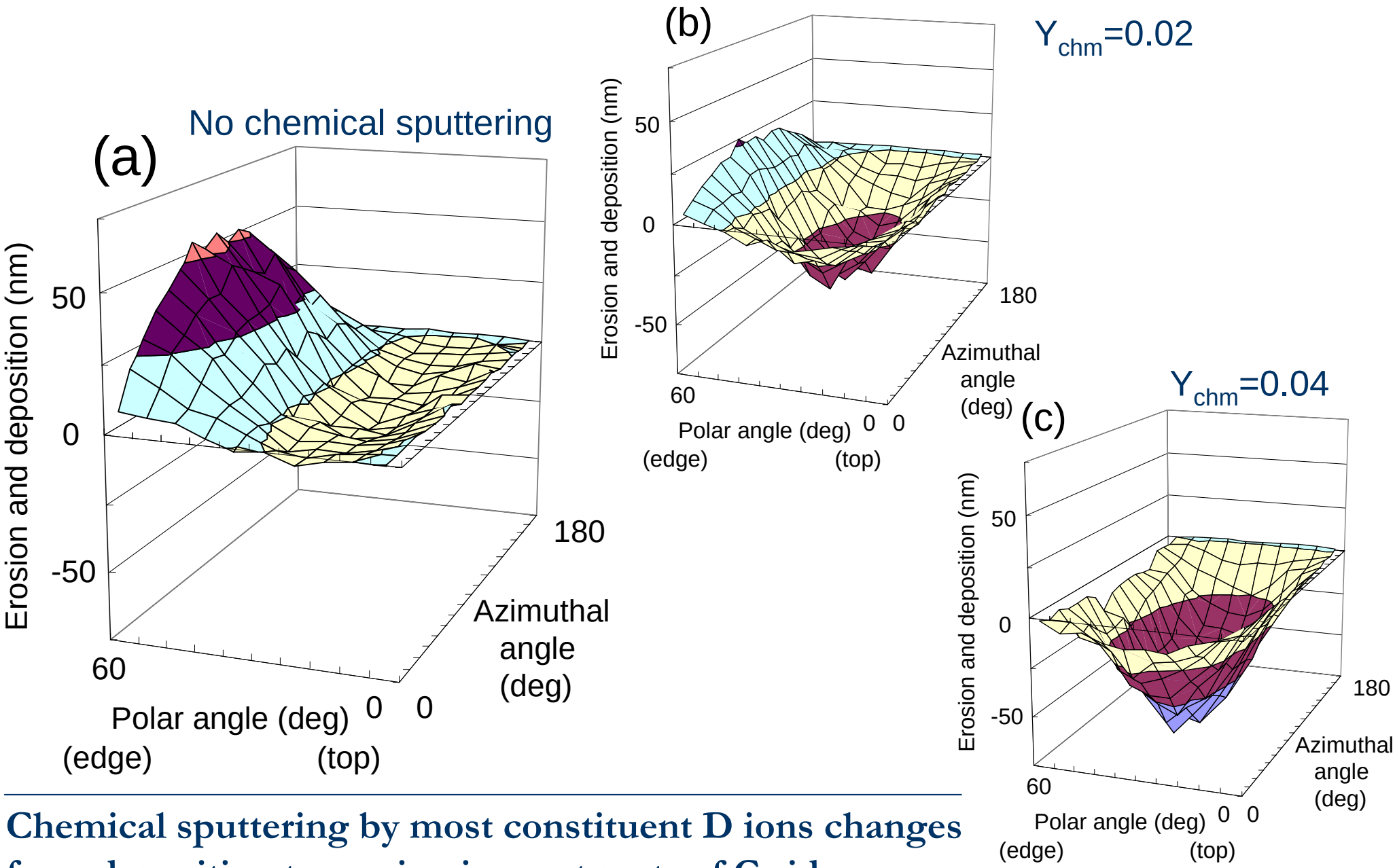


(b) Both erosion and deposition zones appear on W side

(c) A sharp boundary between erosion and deposition zones is produced.



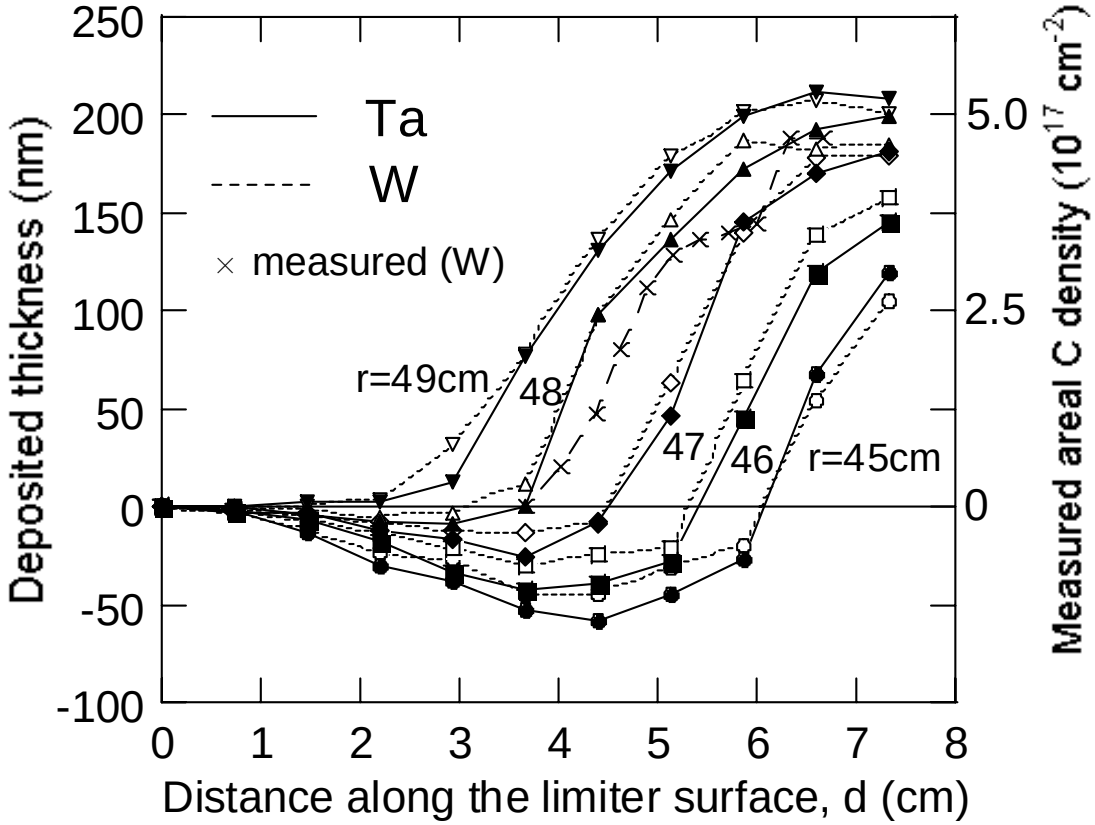
■ Erosion and deposition patterns on C side of W-C twin limiter



Chemical sputtering by most constituent D ions changes from deposition to erosion in most parts of C side.

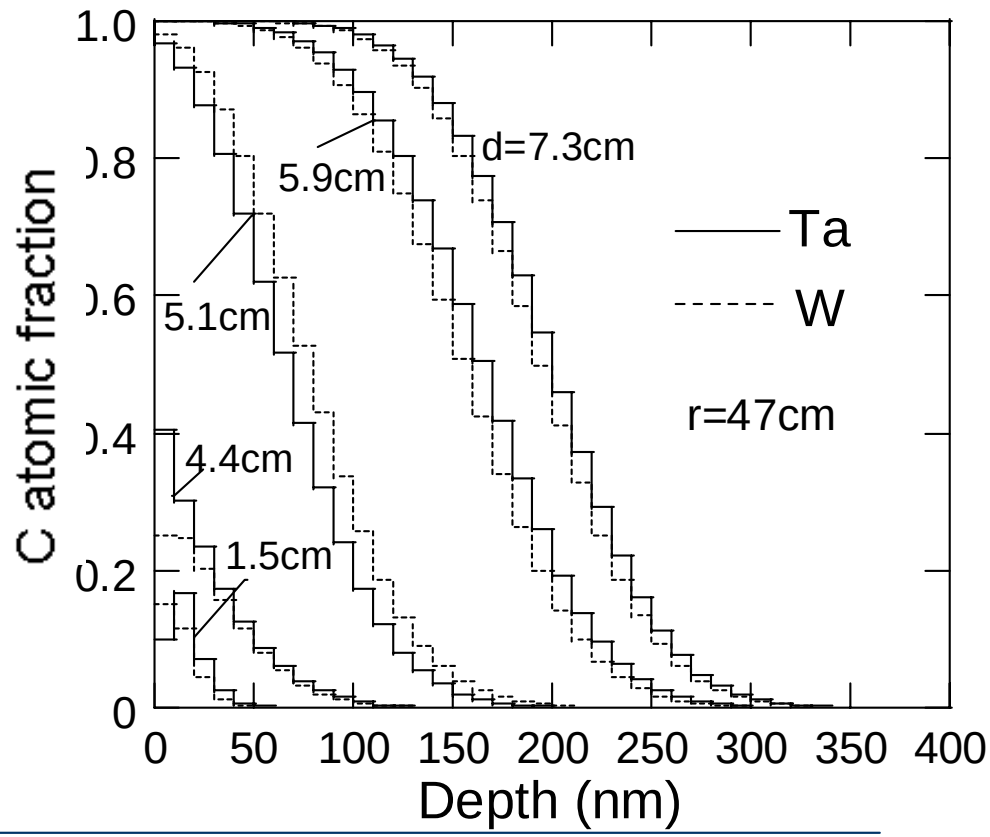
■ Deposited thicknesses on the Ta and W limiters

<no chemical erosion>



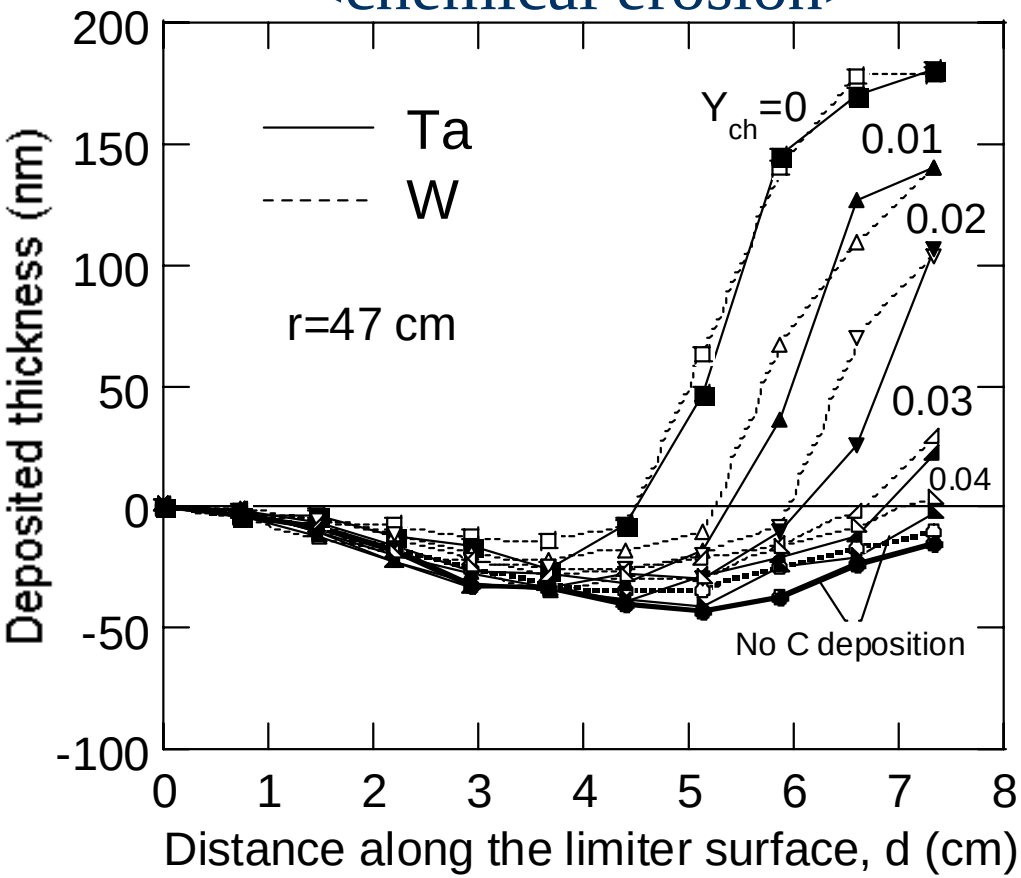
■ Depth profiles of C on the Ta and W limiters

<no chemical erosion>

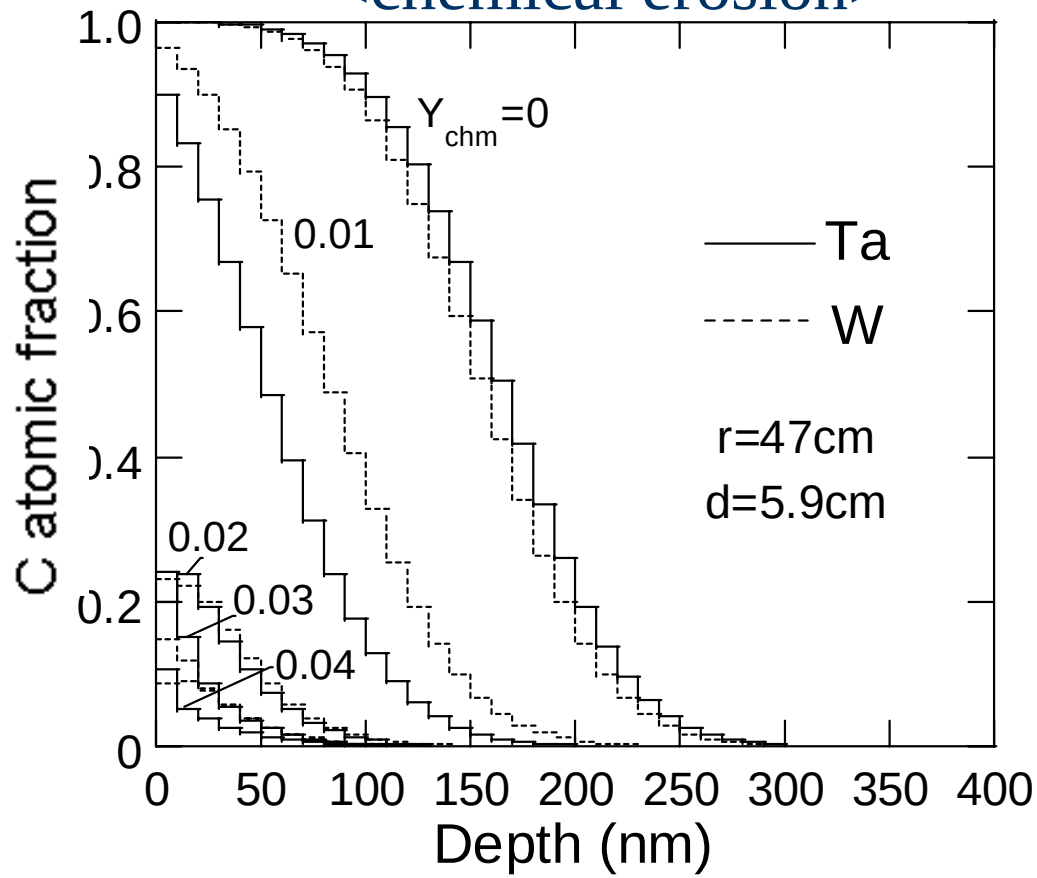


- When approaching the limiter edge, the surface is dominated by strong C deposition, which results in the formation of a thick layer of the deposited C on W and Ta.
- When the limiter is retracted to larger radial distance from the plasma centre, the deposition area broadens towards the top of the limiter.
- Any noticeable difference in the depth profiles of the deposited C between W and Ta is not found.

■ Deposited thicknesses on the Ta and W limiters <chemical erosion>

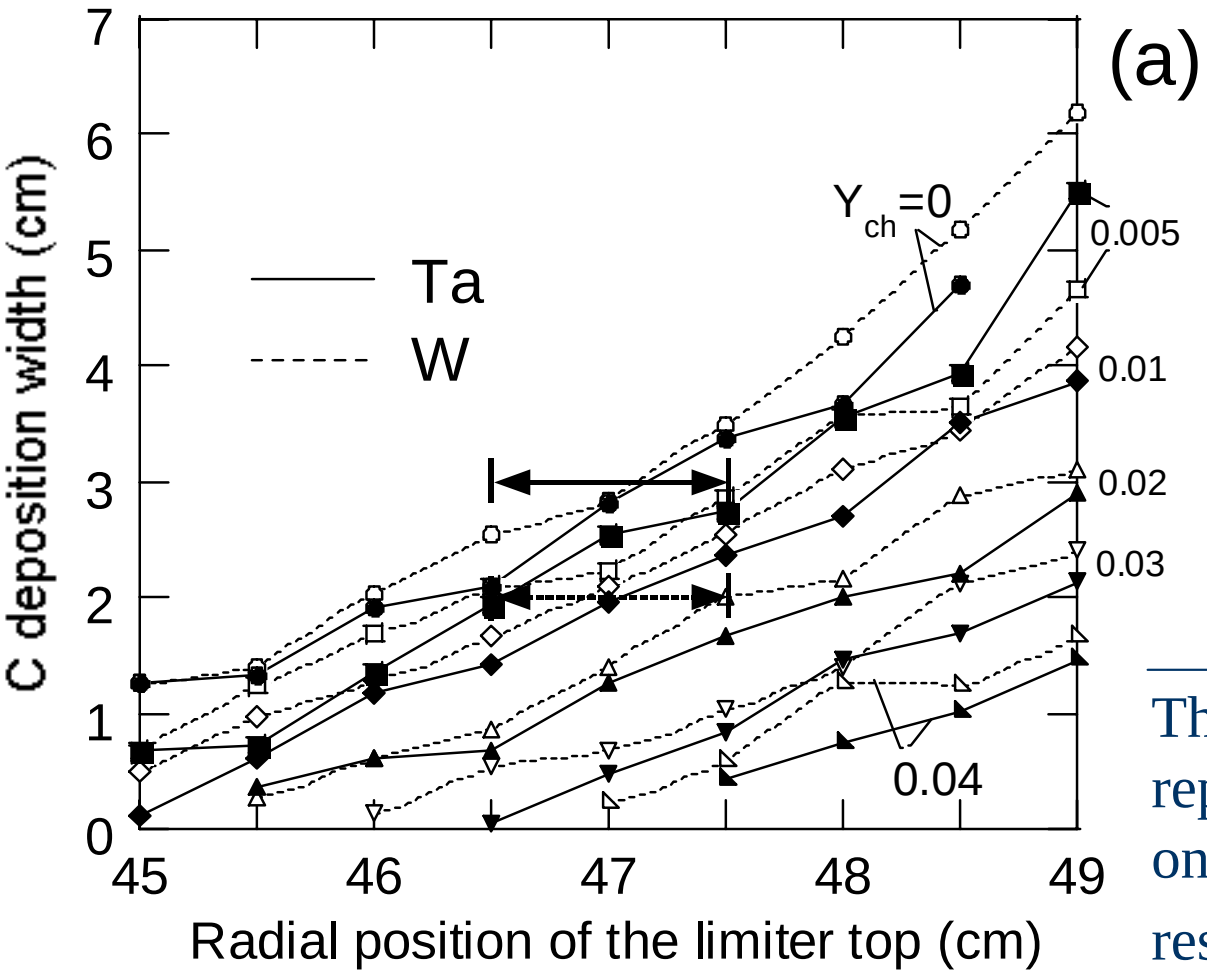


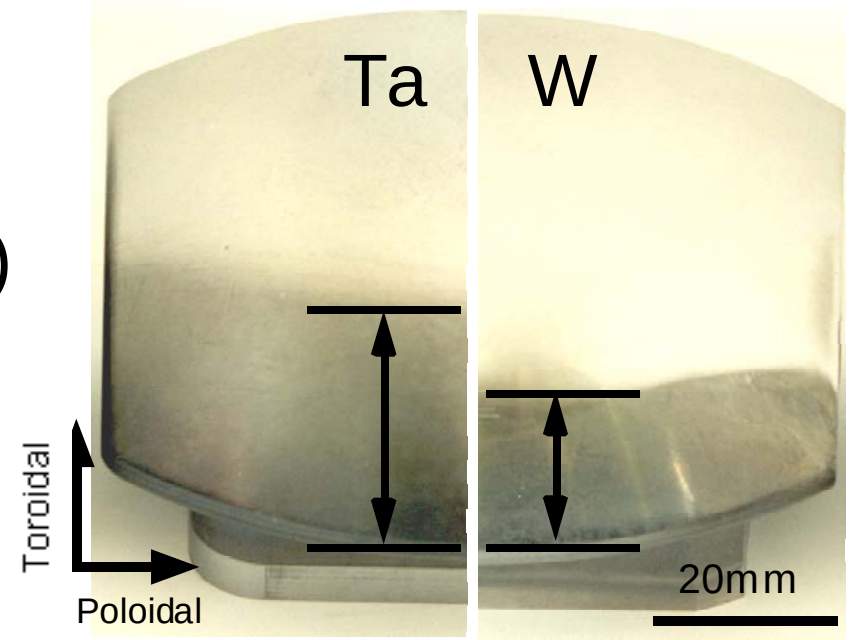
■ Depth profiles of C on the Ta and W limiters <chemical erosion>



- With increasing chemical sputtering yield (Y_{ch}) of the deposited C, the deposition areas tends to be more and more limited to the zone near the limiter edge.
- At high Y_{ch} of 0.04, no deposition is calculated on the whole surface, where W (Ta)-C mixed layers are formed with very small C concentration.
- No difference between W and Ta is calculated if Y_{ch} is the same as for both.

■ Calculated deposition widths for different chemical yields (Y_{ch})





■ View of C deposits on Ta and W parts of the limiter

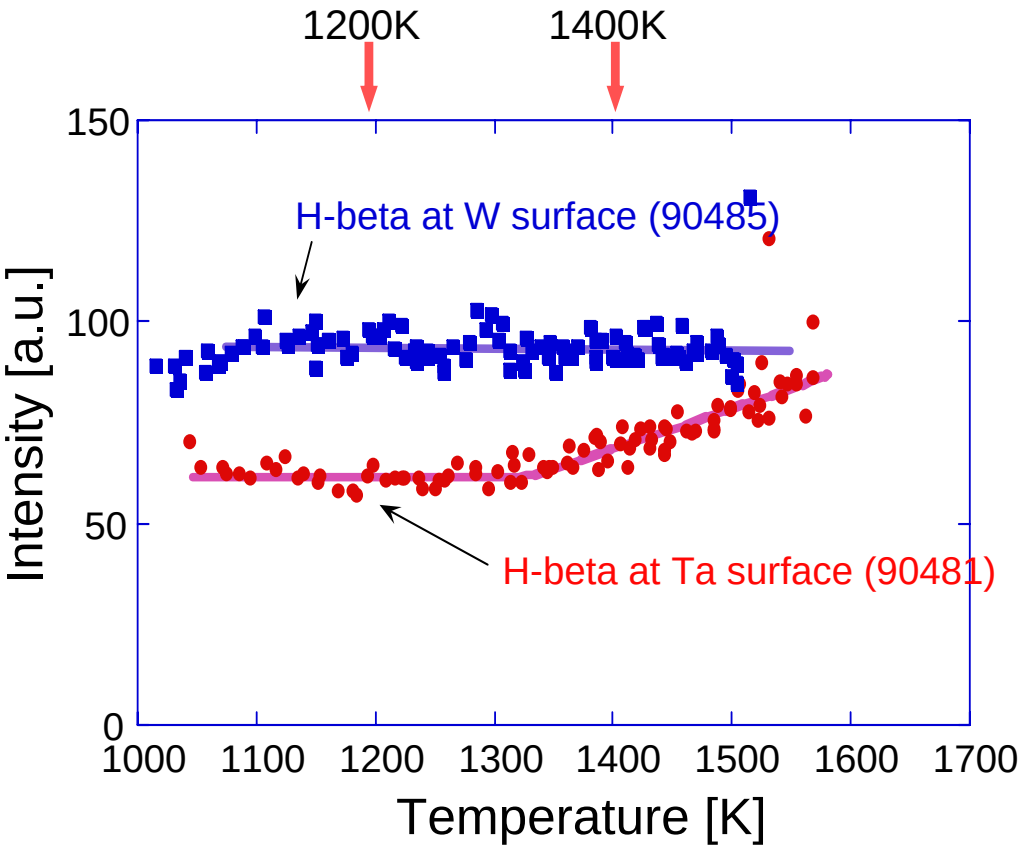
The solid and dotted arrows represent the observed widths on the Ta and W surfaces, respectively.

- Assumptions for chemical erosion yields of ~0.01 for W and <0.005 for Ta fit the calculated widths of the deposition zone to the experimentally determined values.
- The higher surface temperature and higher deuterium trapping rate of Ta are possible reasons for the suppressed chemical erosion of the deposited C on Ta.

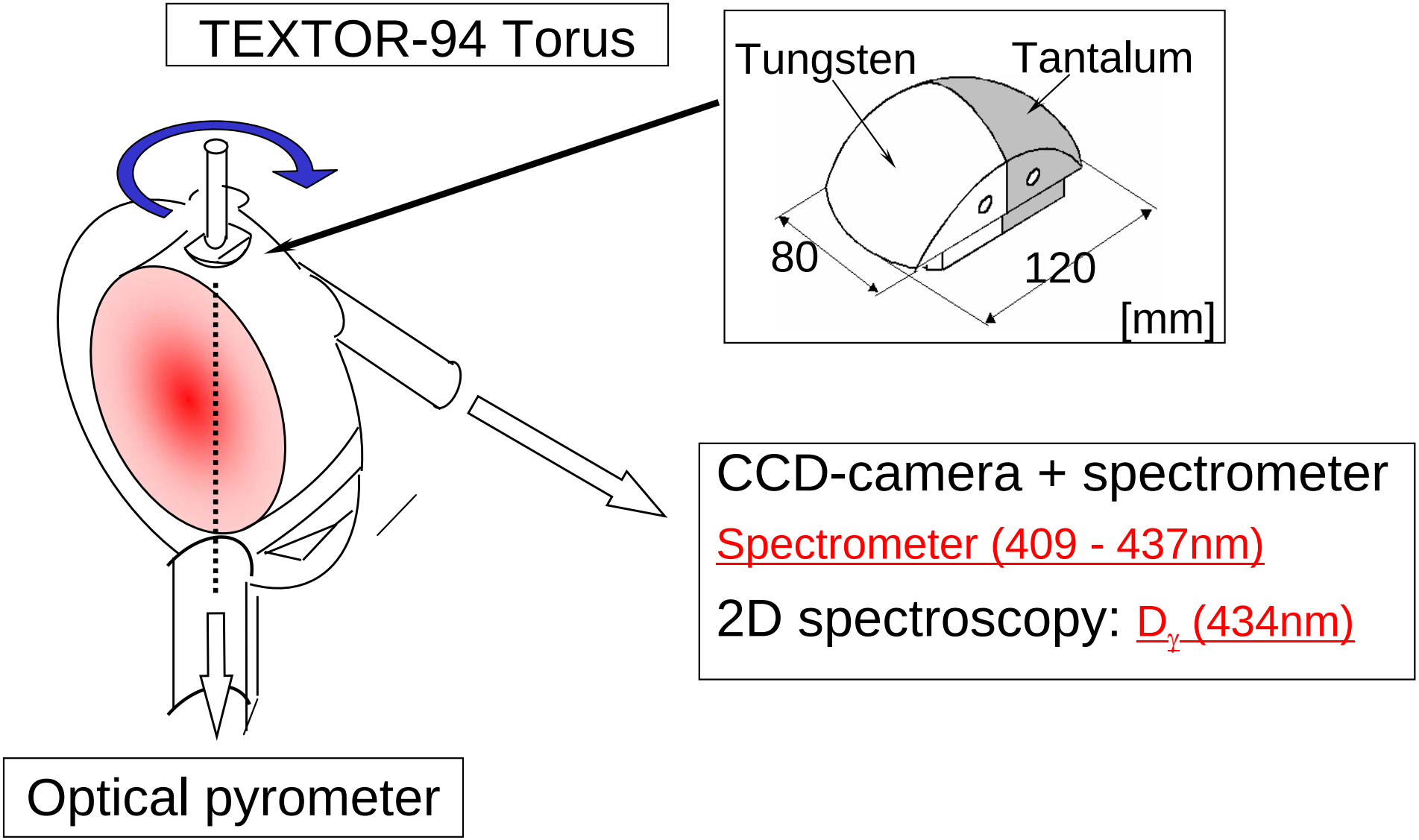
Hydrogen and hydrocarbon release from W and Ta at elevated temperature

- Hydrogen isotopes are released due to different mechanisms from PFCs.
- We have performed a computer simulation of ionisation and dissociation of reflected hydrogen, reemitted atomic and molecular hydrogen, and chemically sputtered hydrocarbon molecules from W and Ta in the plasma.
- The surface temperature and materials dependence of the atomic and molecular fractions of reemitted hydrogen are studied.

- D_β intensity in front of Ta and W as a function of surface temperature during TEXTOR-94 discharges

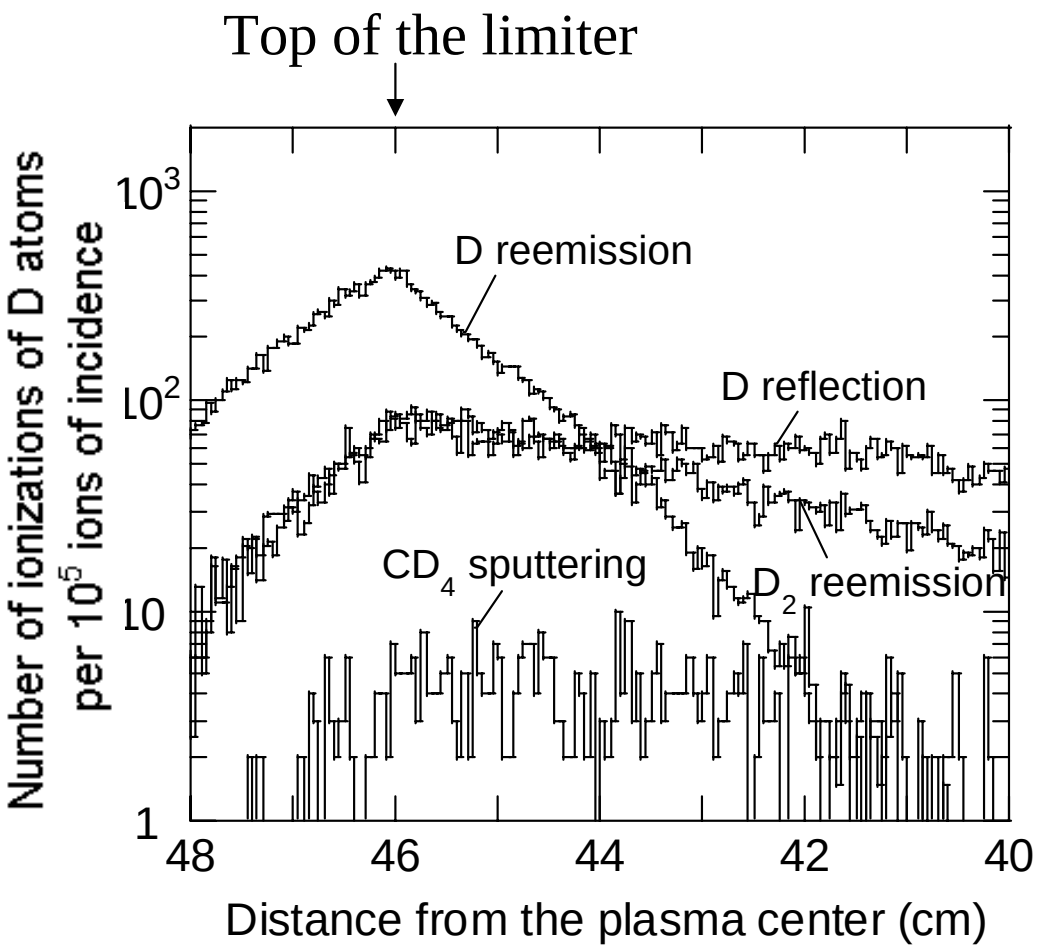


- 2D spectroscopy in W-Ta twin test limiter experiments

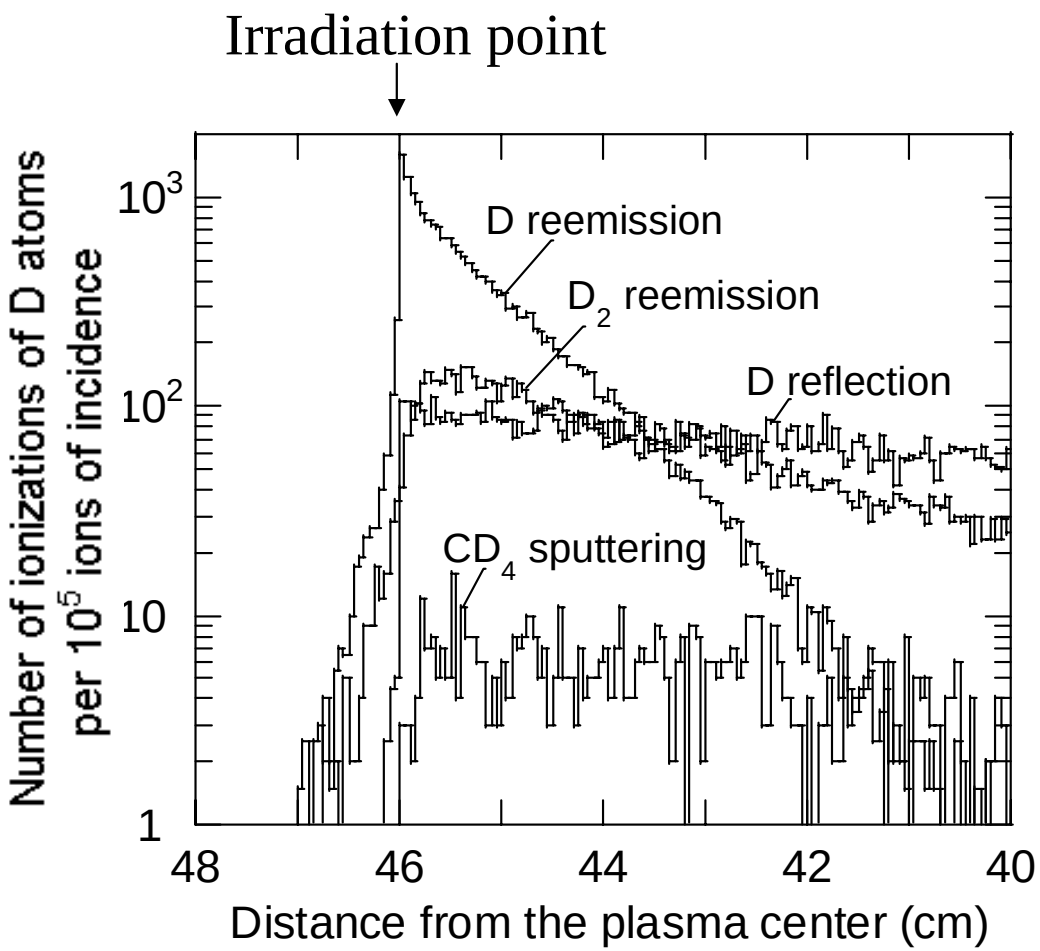


■ Radial distributions of ionizations of reflected and reemitted D from W, and D produced by dissociation after reemission of D_2 and CD_4

<Random irradiation>

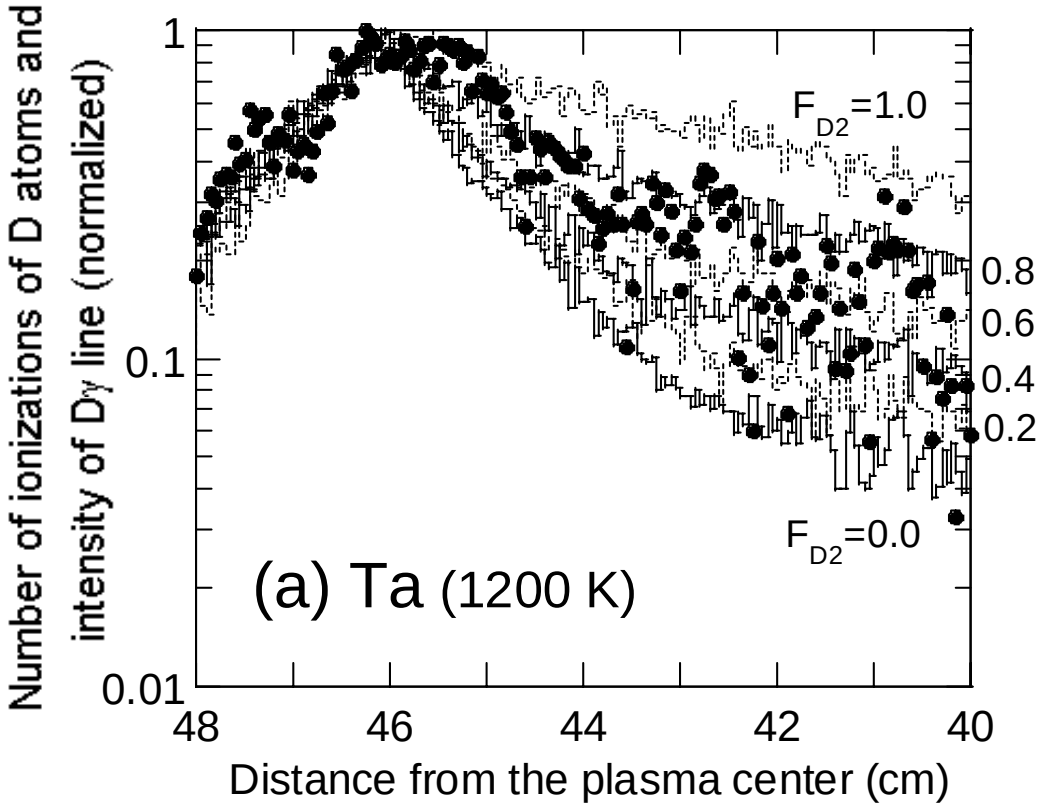


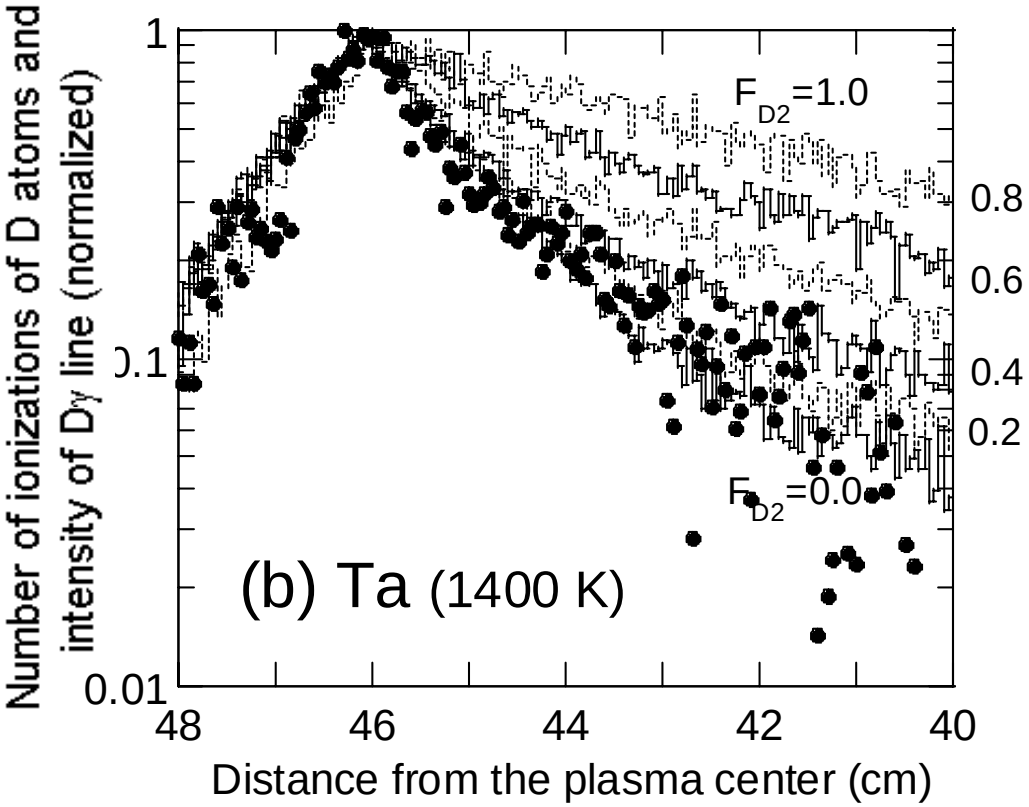
<Fixed point irradiation>



- When the hydrogen is released in the form of hydrogen and methane molecules, different dissociation processes produce the break-up atoms with different energies, which leads to a broad distribution for penetration of D atoms in the plasma.
- A broad distribution behind the top of the limiter (>46 cm), as well in front of it, is influenced by hydrogen release from the whole area of the limiter.

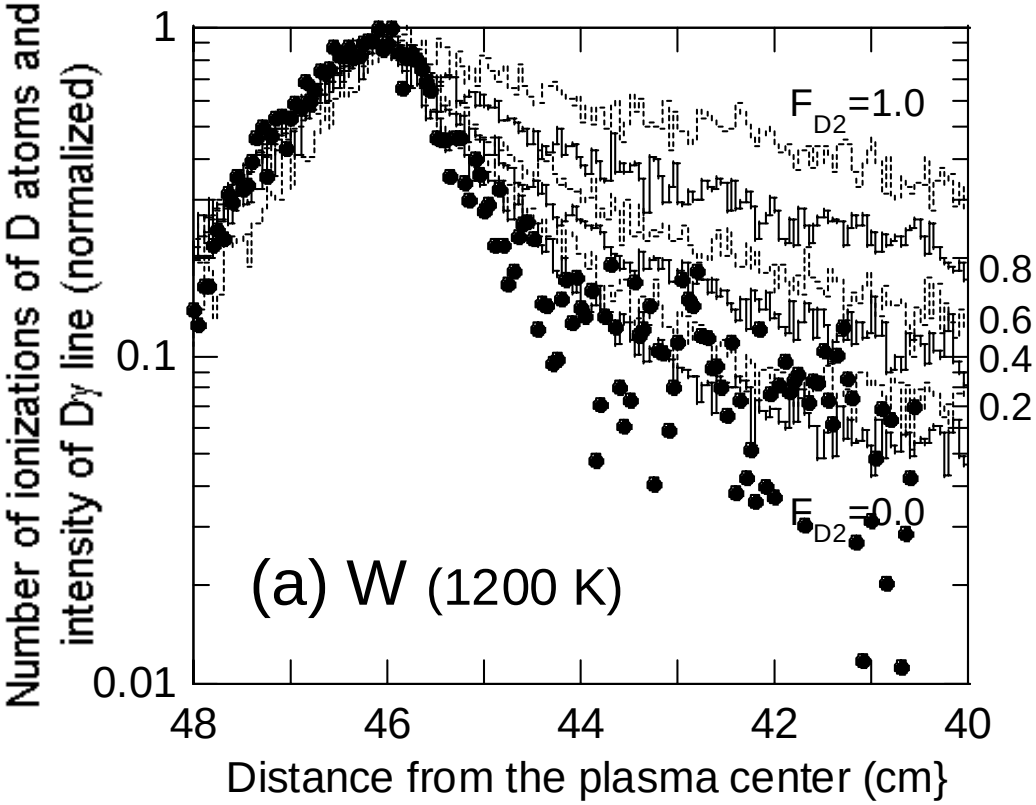
■ Radial distributions of ionizations of D atoms for different molecular fractions and observed distribution of D_γ intensity around Ta

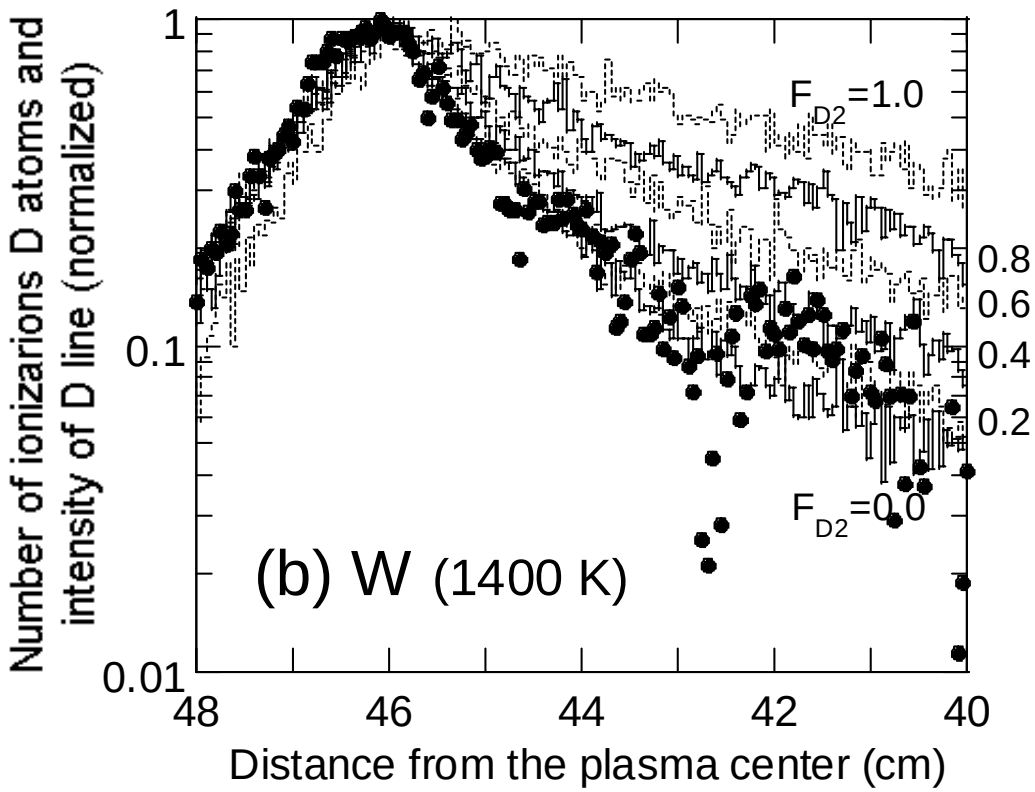




- The calculated distributions are the sum of individual distributions of D atoms, and D_2 and CD_4 molecules which are subsequently dissociated in the plasma.
- The calculated distribution tends to be independent of the surface temperature.
- The observed distributions of D_γ intensities behind the top of the limiter (>46 cm) are reproduced by our calculation due to the bombardment of the whole area of the limiter by plasma ions.

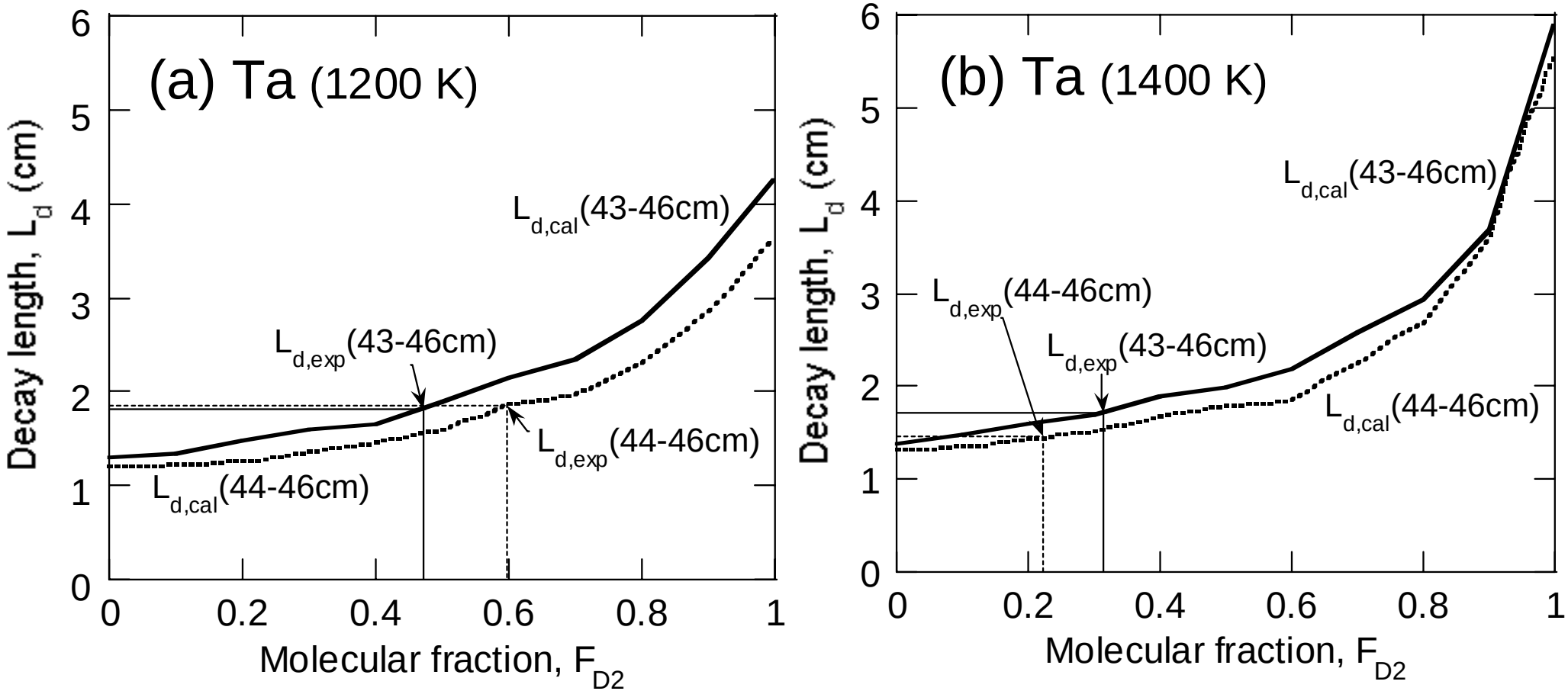
- Radial distributions of ionizations of D atoms for different molecular fractions and observed distribution of D_γ intensity around W





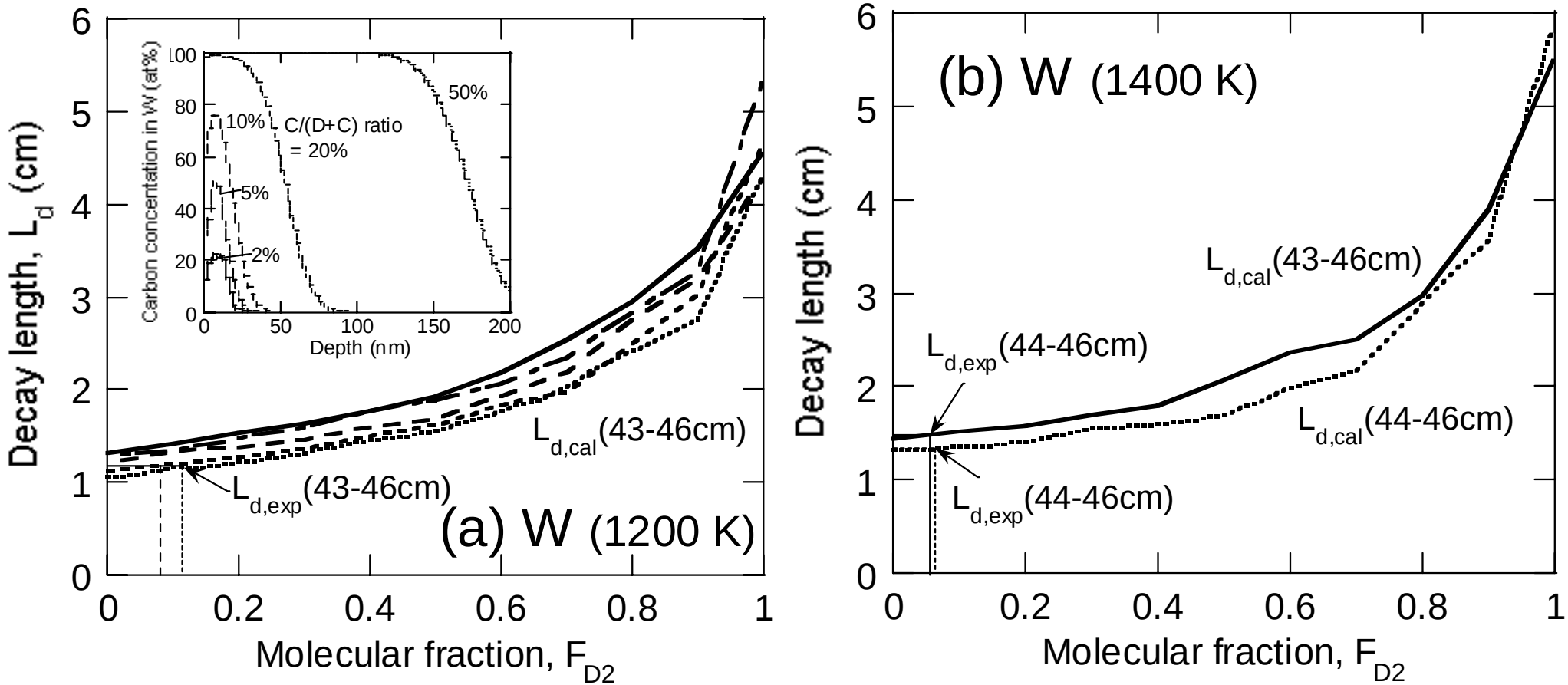
- The observed D_γ distribution around the limiter can be fitted to the calculated distribution with a given molecular fraction.
- It allows us to estimate the atomic and molecular fractions in the reemitted hydrogen from the limiter.
- To reduce the influence of the scatter in the observed distribution when fitting to the calculation, decay lengths for both distributions are determined.

- Decay length of ionizations of D atoms as a function of the molecular fraction from Ta and decay length of observed distributions



- For hydrogen reemission from Ta at 1200 K, the atomic and molecular hydrogens are comparable to each other: the molecular fraction, F_{D2}=0.46~0.60, whereas the molecular fraction decreases with increasing temperature: at 1400 K, F_{D2}=0.22~0.31.
- This change in molecular fraction with the surface temperature is similar to that in the case of graphite.

■ Decay length of ionizations of D atoms as a function of the molecular fraction from W and decay length of observed distributions



- For W, most of hydrogen are reemitted in the form of atoms for both temperatures: F_{D2}~0 at 1200 K and F_{D2}~0.05 at 1400 K.
- The reason for the dominant reemission of atomic hydrogen at such low surface temperature is not clearly understood, but it seems to be explained with high flux irradiation of hydrogen ($<5\times10^{22}D^+/m^2s$) and endothermic property of W for hydrogen.

Redeposition patterns of hydrocarbons in the gaps between divertor tiles

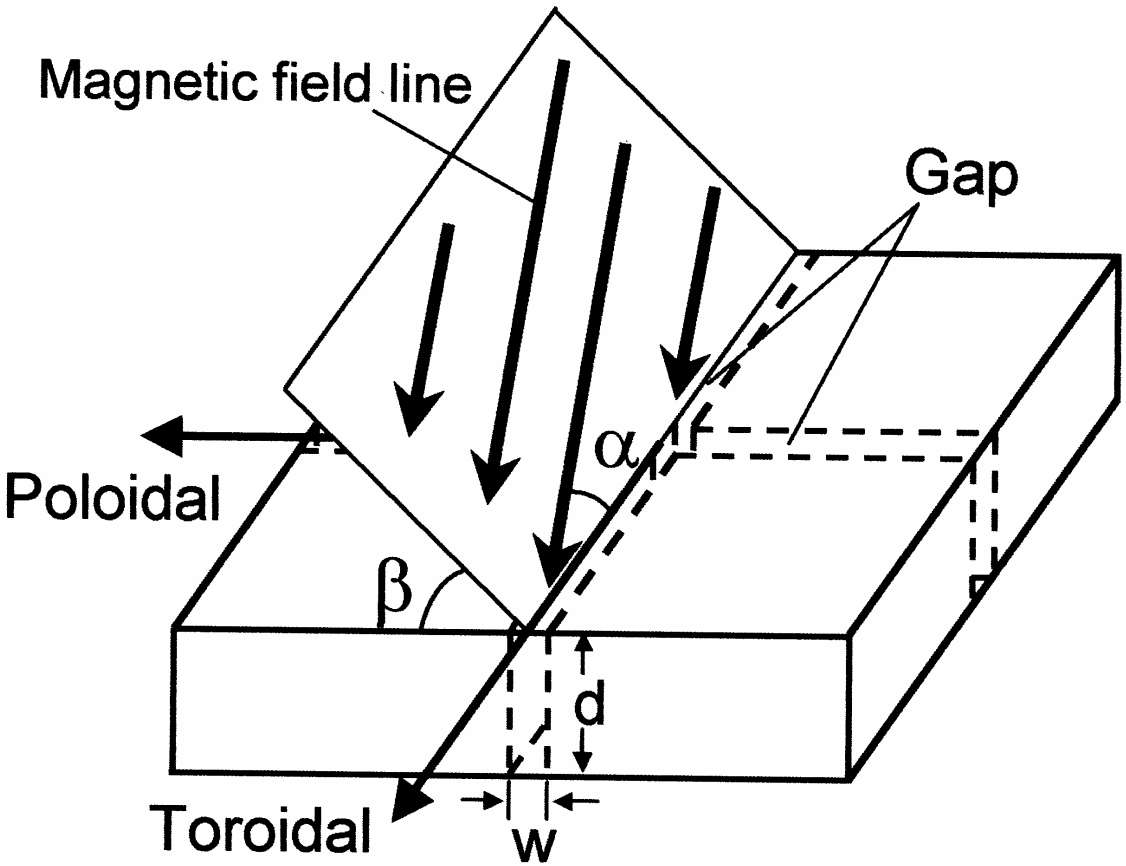
- Hydrocarbon molecules produced by the chemical erosion redeposit on graphite divertor tiles after migration in edge plasmas. The tritium retention is dominated by the inventory retained in the deposited hydrocarbon layers on the components.

- Transport of various hydrocarbons, i.e., CH_4, C_2H_2, C_2H_4, C_2H_6 and C_3H_6, in divertor plasmas and their redeposition on a wall surface are investigated by computer simulations in terms of plasma temperature and density.

- Recent surface analyses of the used tiles have revealed thick deposited layers with high tritium concentration on the tile sides and gaps between the tiles.

- We attract our attention on the spatial distribution of carbon and hydrocarbons deposited in the gaps in the toroidal and poloidal directions

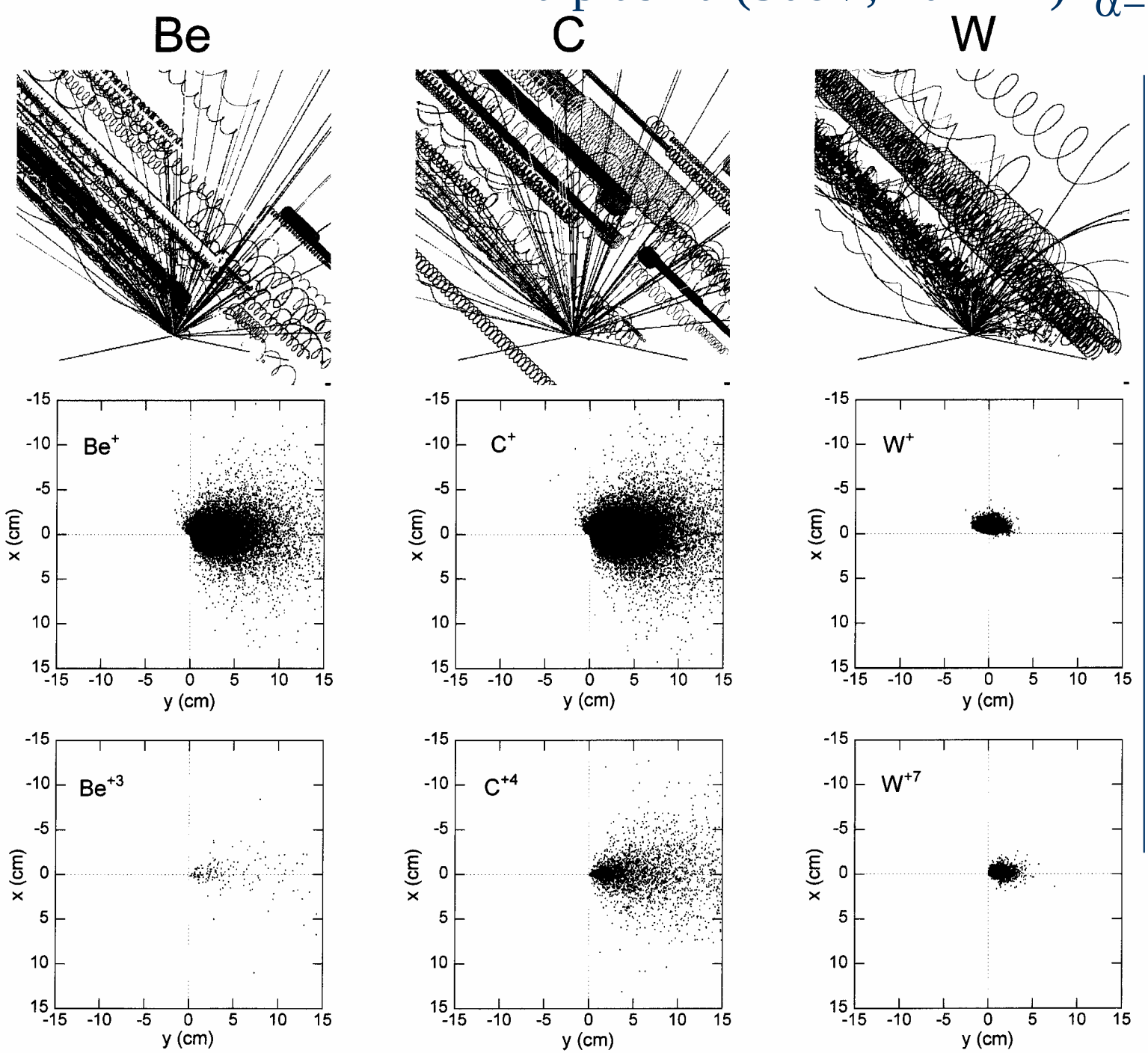
■ Simple geometries of a divertor tile and toroidal and poloidal gaps between the tiles



- A homogeneous plasma with constant electron and ion temperatures, T_e and T_i (T_e=T_i), and the constant electron density, n_e, contacts the tile surface.
- The neutral atoms physically sputtered undergo successive ionisations by plasma electrons and gyrate in an oblique magnetic field.
- Possible reactions for hydrocarbons are electron-impact ionisations, dissociations and dissociative recombinations and proton-impact ionisations and charge exchange processes of the hydrocarbons.
- For redeposition on the sides of the tiles and gaps between the tiles, a simple model of toroidal and poloidal gaps with the width, *w*, and the depth, *d*, is used.

■ Trajectories and redeposition patterns of sputtered Be, C and W in a plasma (30eV, $10^{19}m^{-3}$)

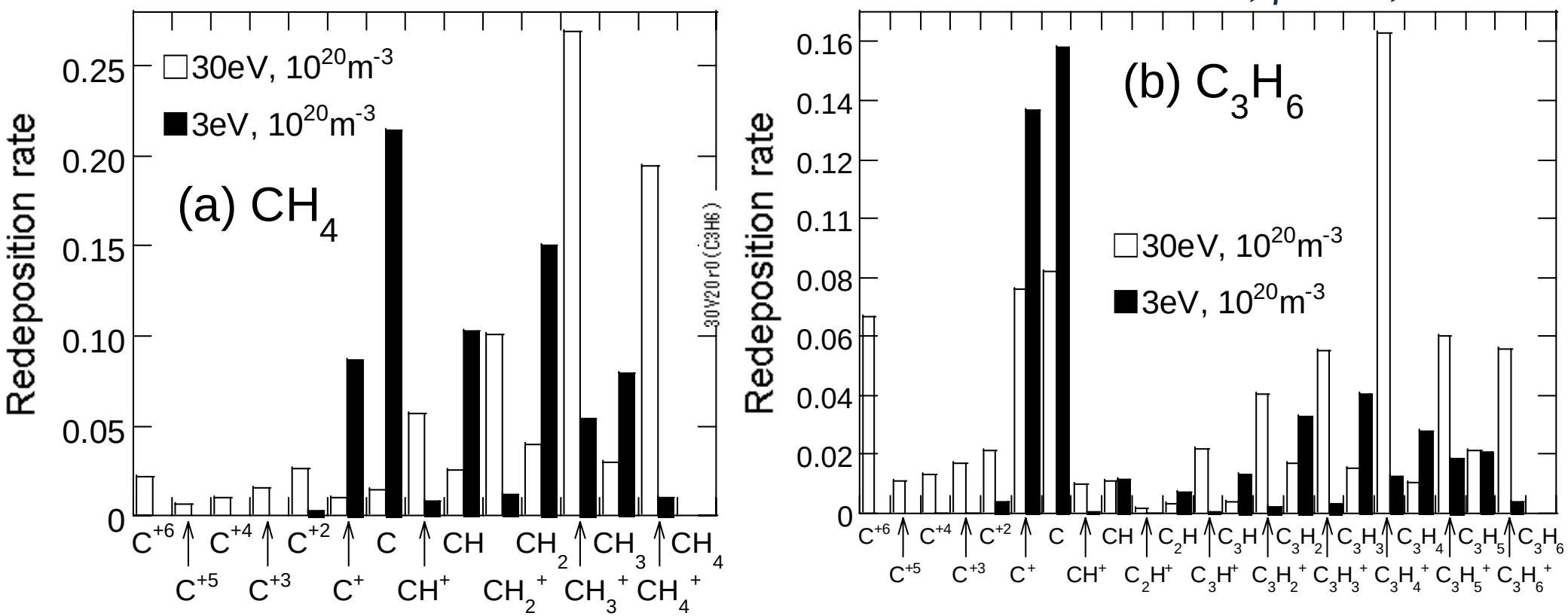
$\alpha = 30^o$, $\beta = 90^o$, B=2 T



- Due to prompt redeposition of singly ionised W,redeposition patterns of W is asymmetric in dependent of the turning point of gyromotion in the plasma.
- The patterns are much more localized than those of C and Be where the ionised C and Be move along the magnetic field lines before redeposition.

■ Carbon and hydrocarbon redeposited species on the tile surface for the release of (a) CH_4 and (b) C_3H_6 in plasmas

$\alpha = 5^o$, $\beta = 30^o$, B=5 T

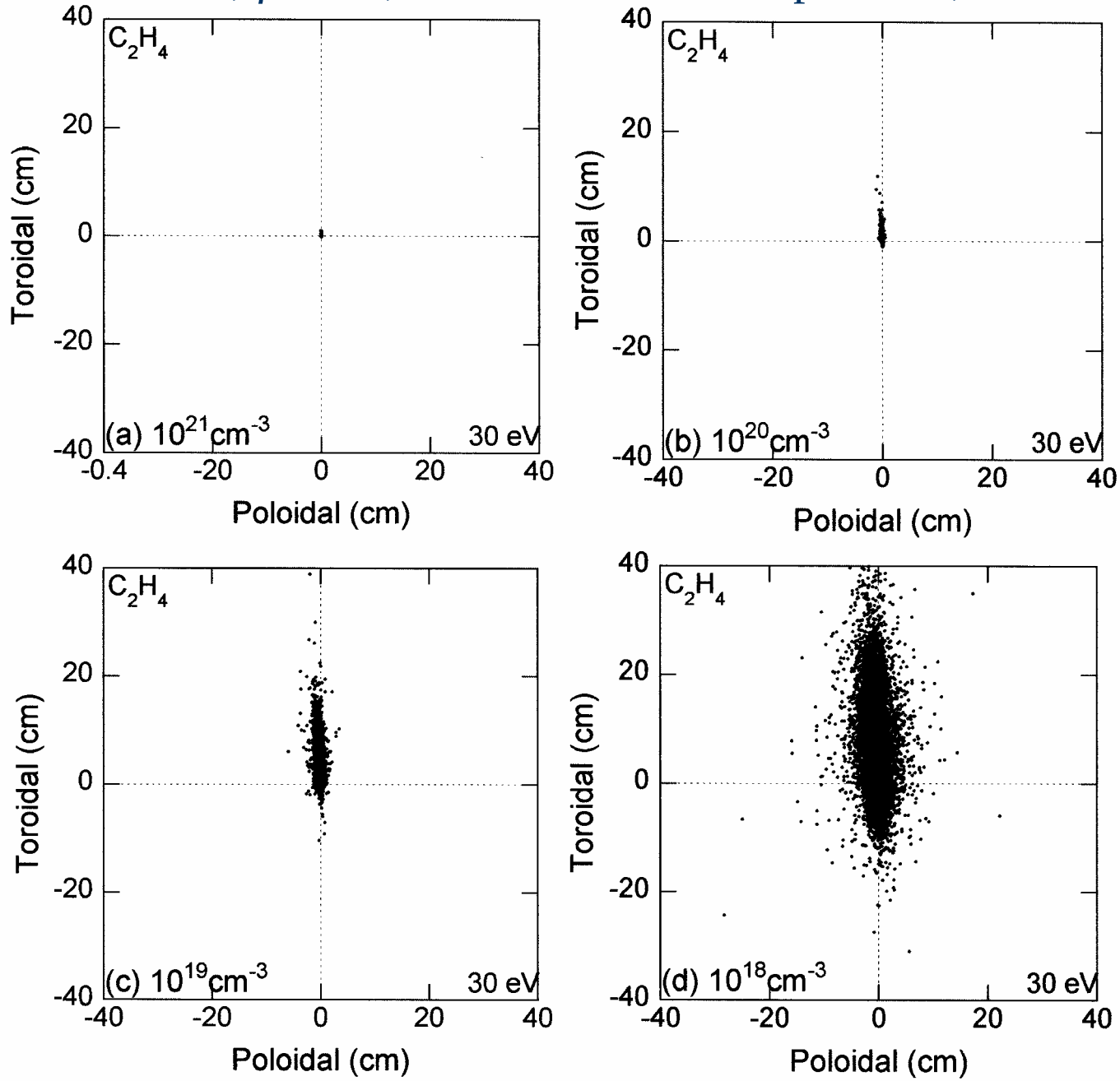


- The redeposition spectrum is more complex for C_3H_6 than for CH_4.
- A much higher neutral fraction is redeposited at low temperature, due to a reaction chain of proton-impact ionisation and electron-impact dissociative recombination.
- At high temperature, electron-impact ionisation accompanied with dissociation produces dominant ion fragments.

■ Redeposition patterns of carbon and hydrocarbon fragments for the release of C_2H_4 molecules in the plasmas

α= 5° , β=30° , B=5 T Plasma temperature; 30 eV

- The released position is the centre of the tile surface.
- For high-density and high-temperature plasmas, the patterns are extremely small due to dominant electron-impact ioinisation just after the release.
- With decreasing plasma density, the redeposition patterns largely broaden towards the toroidal direction, because the ionisation events occur deeply in the plasma and the ionised particles move along the magnetic field lines.

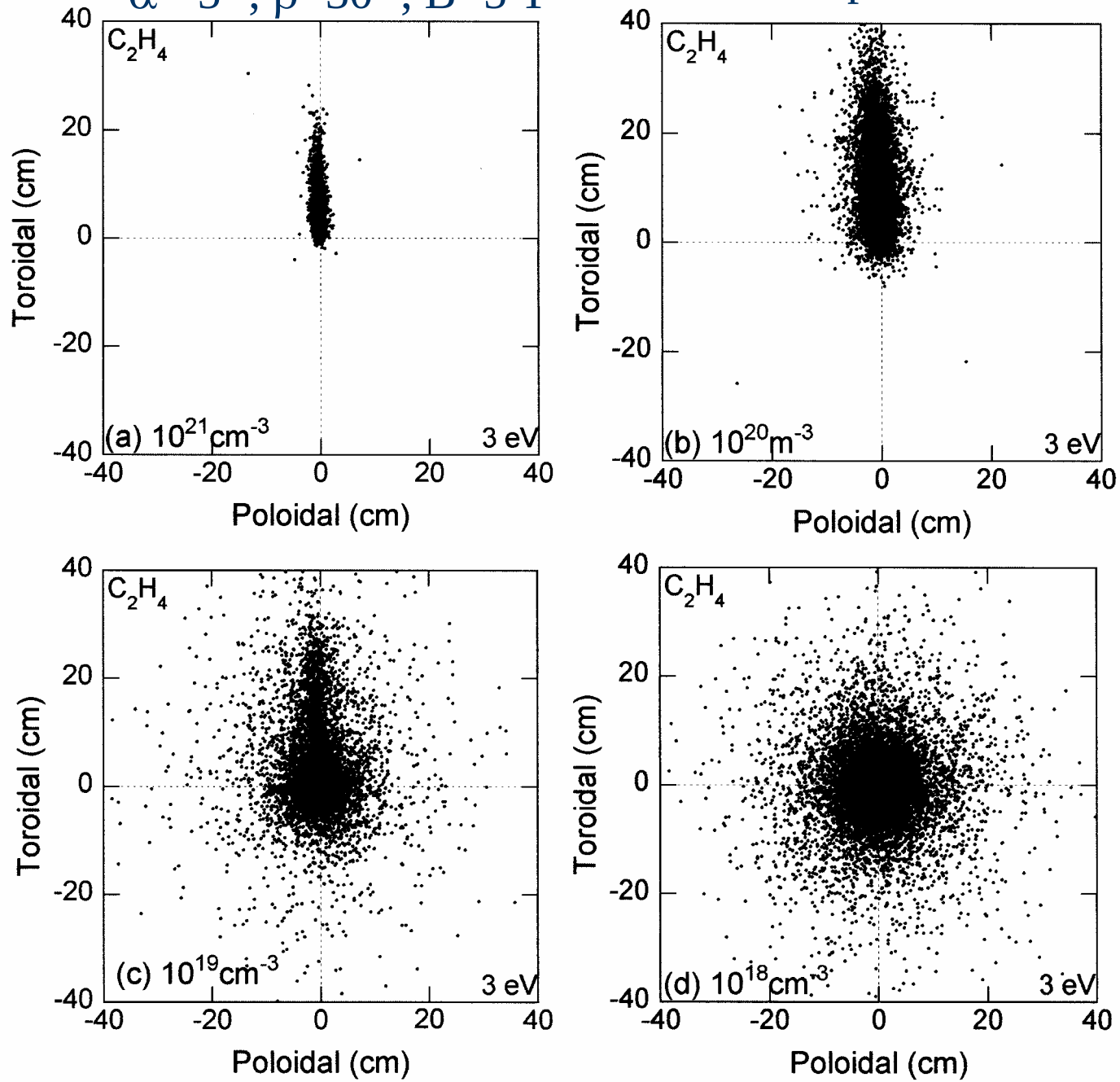


■ Redeposition patterns of carbon and hydrocarbon fragments for the release of C_2H_4 molecules in the plasmas

$\alpha = 5^o$, $\beta = 30^o$, B=5 T

Plasma temperature: 3 eV

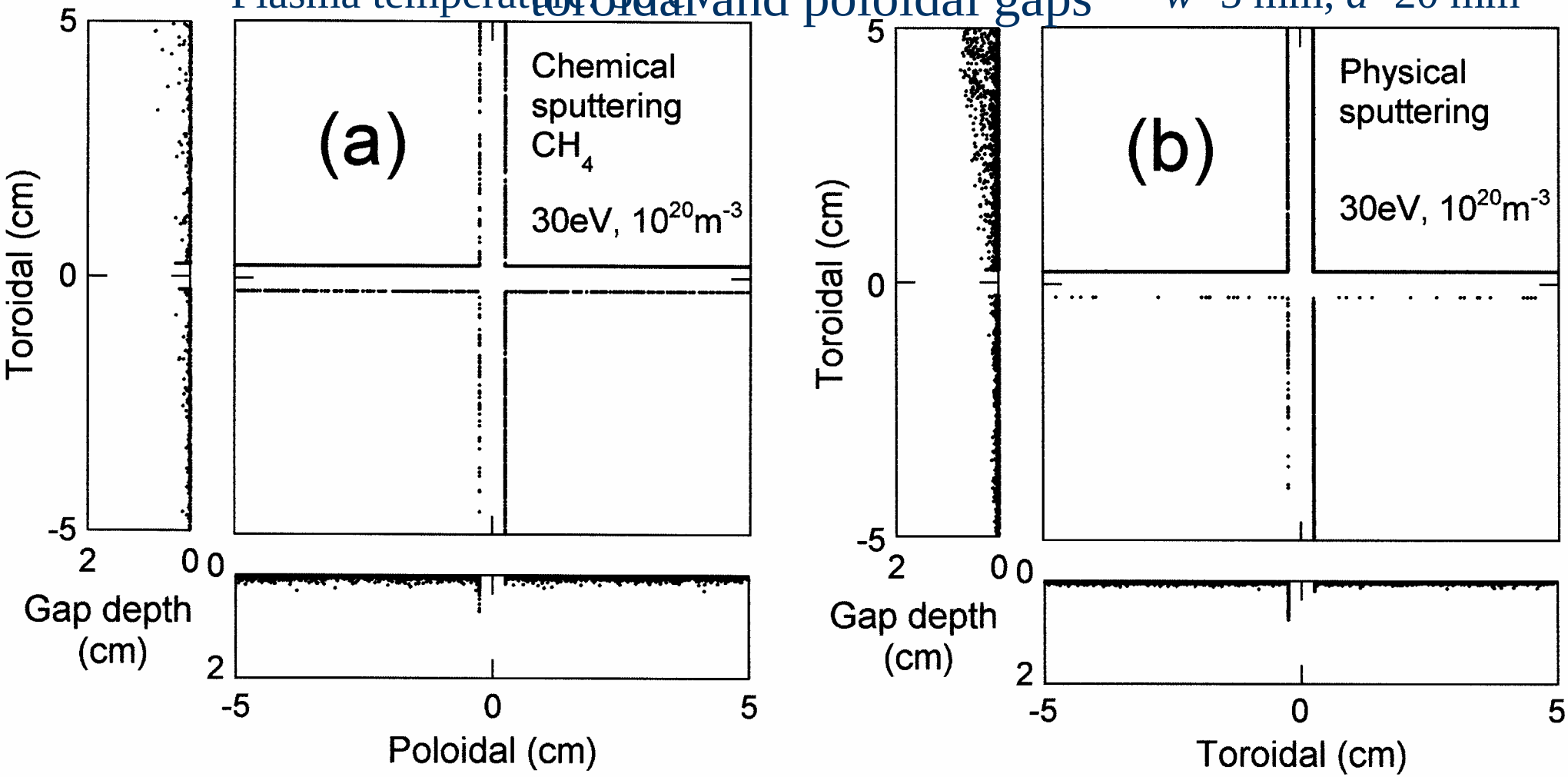
- Hydrocarbon penetration into the plasma is greater at low temperature where much less type of reactions can occur.
- With decreasing plasma density, hydrocarbons penetrates more deeply into the plasma, and as a result, the redeposition patterns broadens more and more in the poloidal and toroidal directions.
- For low-temperature (3eV) and low-density ($10^{18}cm^{-3}$) plasmas, the redepositions distribute over several tens of cm.



■ Redeposition patterns of carbon and hydrocarbon fragments in toroidal and poloidal gaps

Plasma temperature: 30 eV

$\alpha = 5^o$, $\beta = 30^o$, B=5 T
w=5 mm, d=20 mm

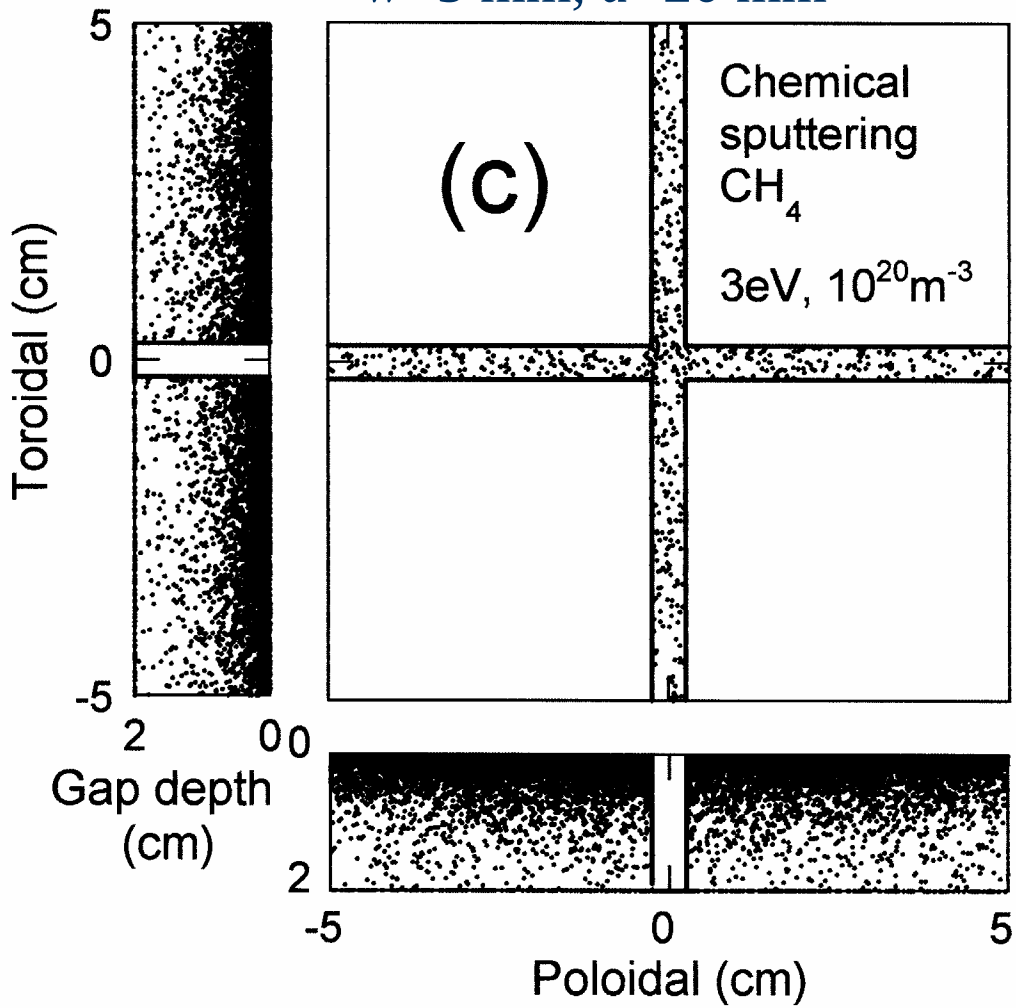


- At high plasma temperature, the redeposition is observed only on the shallow side in the gap and there is no redeposition on the bottom or the inner part of the gap.
- There is asymmetry in the redeposition patterns between toroidal and poloidal gaps.
- The patterns are dominated by the magnetic geometry on the tile surface, which are very similar to the redeposition patterns of physically sputtered carbons

■ Redeposition patterns of carbon and hydrocarbon fragments in toroidal and poloidal gaps

Plasma temperature: 3 eV

$\alpha = 5^o$, $\beta = 30^o$, B=5 T
w=5 mm, *d*=20 mm



- Neutral species are liberated from a magnetic constrain and as a result, they randomly deposit not only on the top surface of the tiles but also in the bottom and the inner part of the gap between the tiles.
- There is no asymmetry in the redeposition patterns between the toroidal and poloidal gaps.
- Since the bottom and the inner part of the gaps are not contacted by the plasma, the hydrocarbons deposited in the gap remain for a long time.
- Due to successive deposition of hydrocarbons, a thick carbon deposition layer may be formed at the sides of the tile and the gaps between the tiles, as observed in present large tokamaks.

Thank you very much

for your attention