Impact of gyro-motion and sheath acceleration on the flux distribution on rough surfaces

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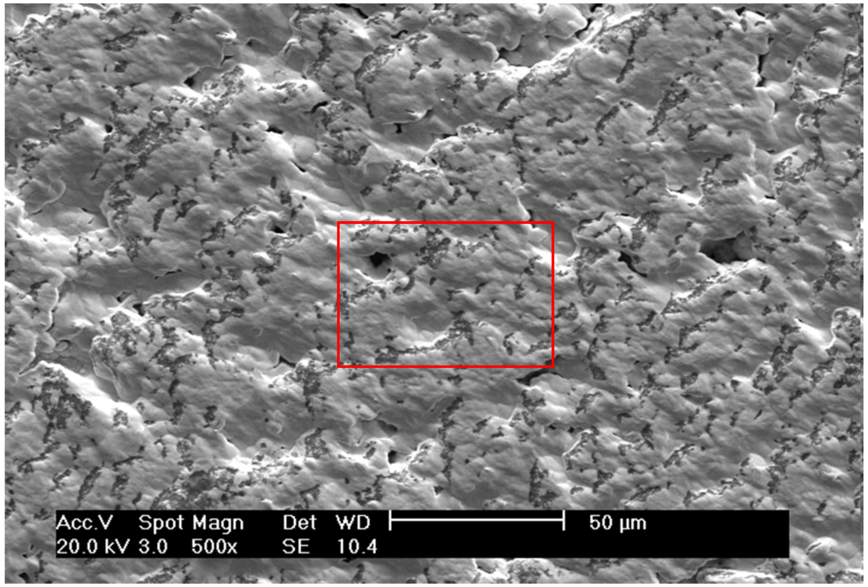
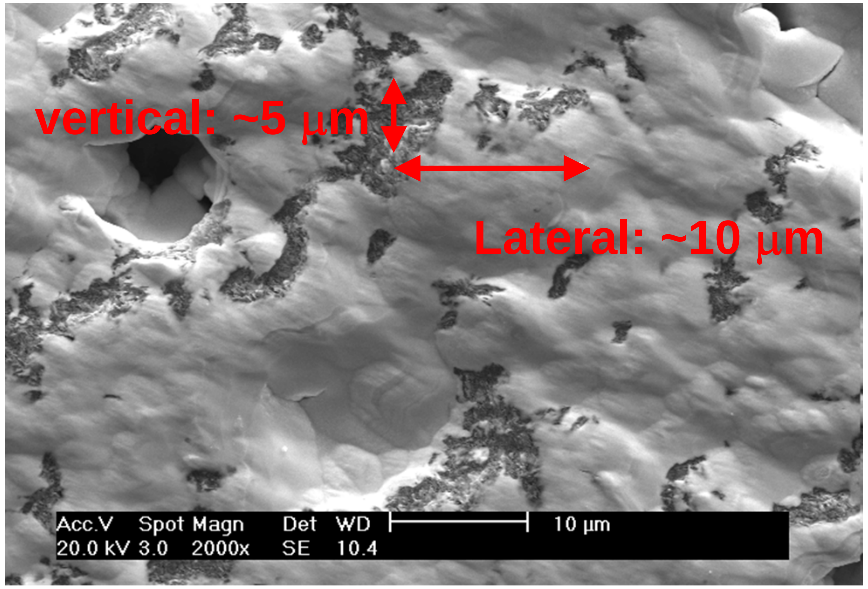
Outline

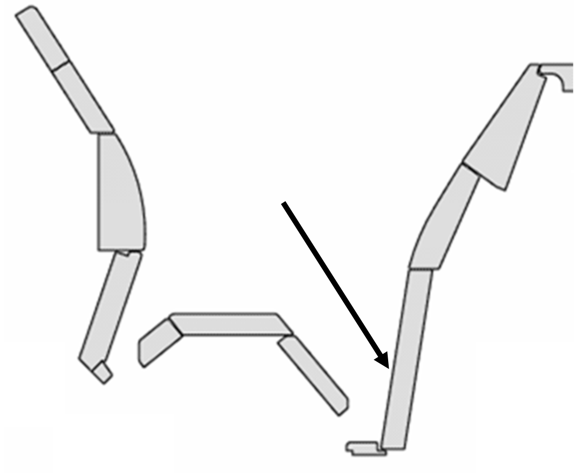
- Introduction
- Experimental erosion patterns on W coated C
- Modeling particle trajectories in the sheath
- Impact angle distributions
- Variation of flux across rough surfaces
- Erosion distributions on real surfaces
- Summary

Introduction





Inhomogeneous erosion of W in AUG
(M. Mayer PFMC 2009)



Initial: 1.5 µm W
Mean erosion: 0.28 µm
Max erosion: > 1.5 µm

Very inhomogeneous erosion of marker

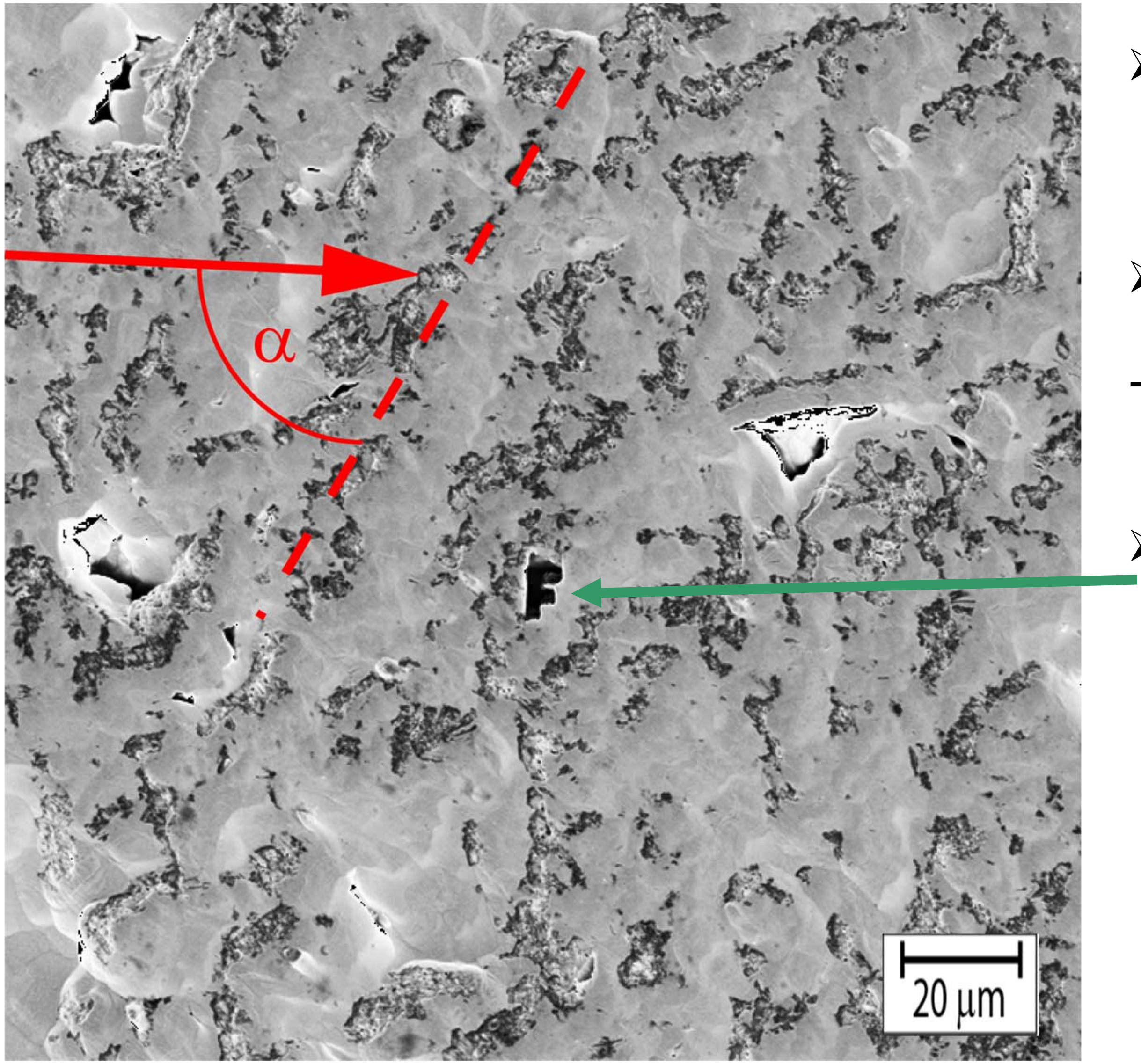
⇒ Larger local erosion on plasma-exposed surfaces than mean

⇒ Some W deposition in shadowed areas

➢ **Why is that so ?**

Experimental erosion patterns on W coated C

❖**SEM image of eroded AUG tile from outer divertor**



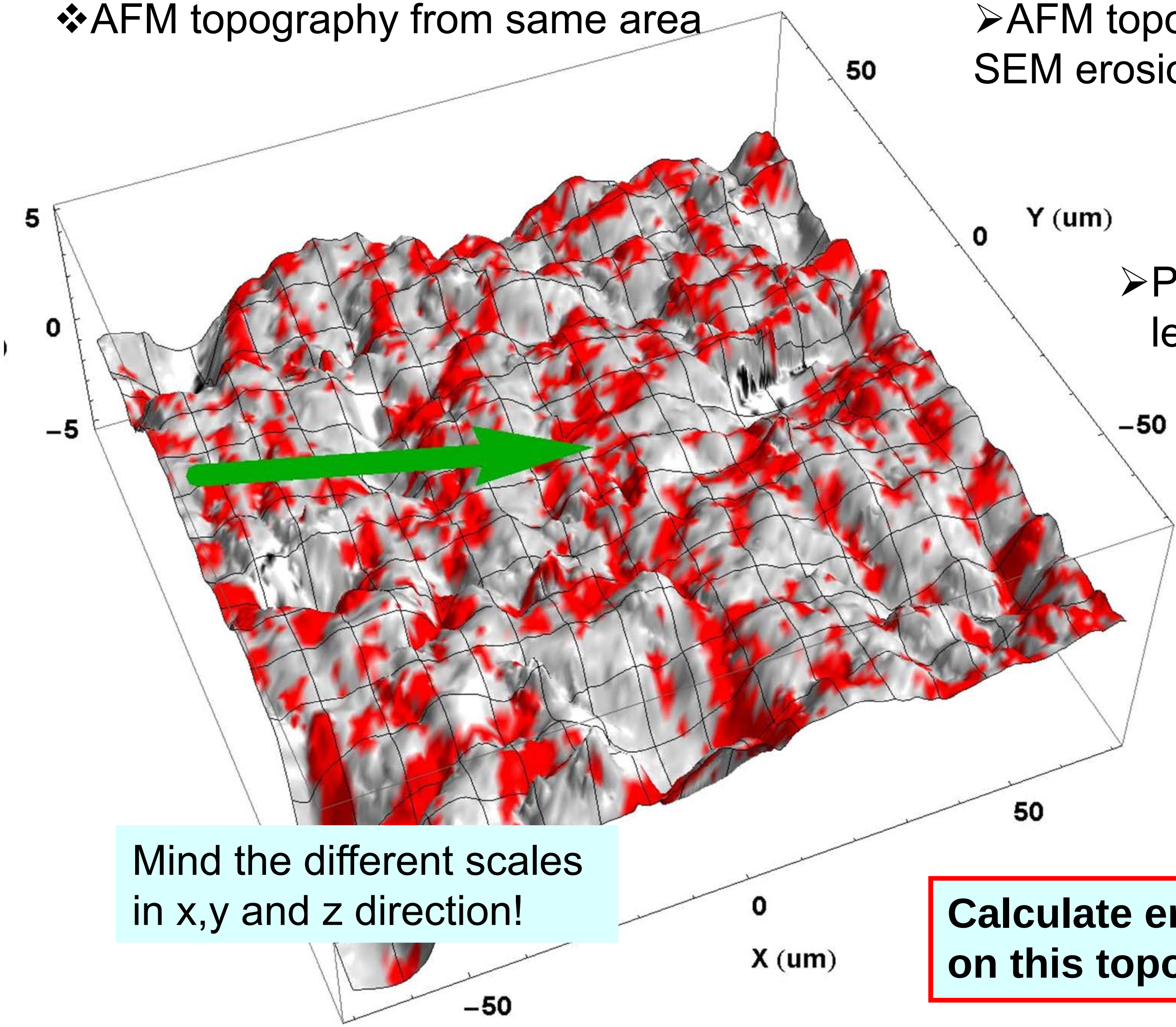
- ➢Inhomogeneous erosion pattern
- ➢Angle α≠90° between eroded ridges and B-Field
  → Hints towards ExB effect
- ➢Location marked by letter F in FIB

Experimental erosion patterns on W coated C

❖AFM topography from same area

➢AFM topography overlaid by SEM erosion pattern (red)

➢Pronounced erosion on leading edges



Mind the different scales in x,y and z direction!

Calculate erosion flux distribution on this topography

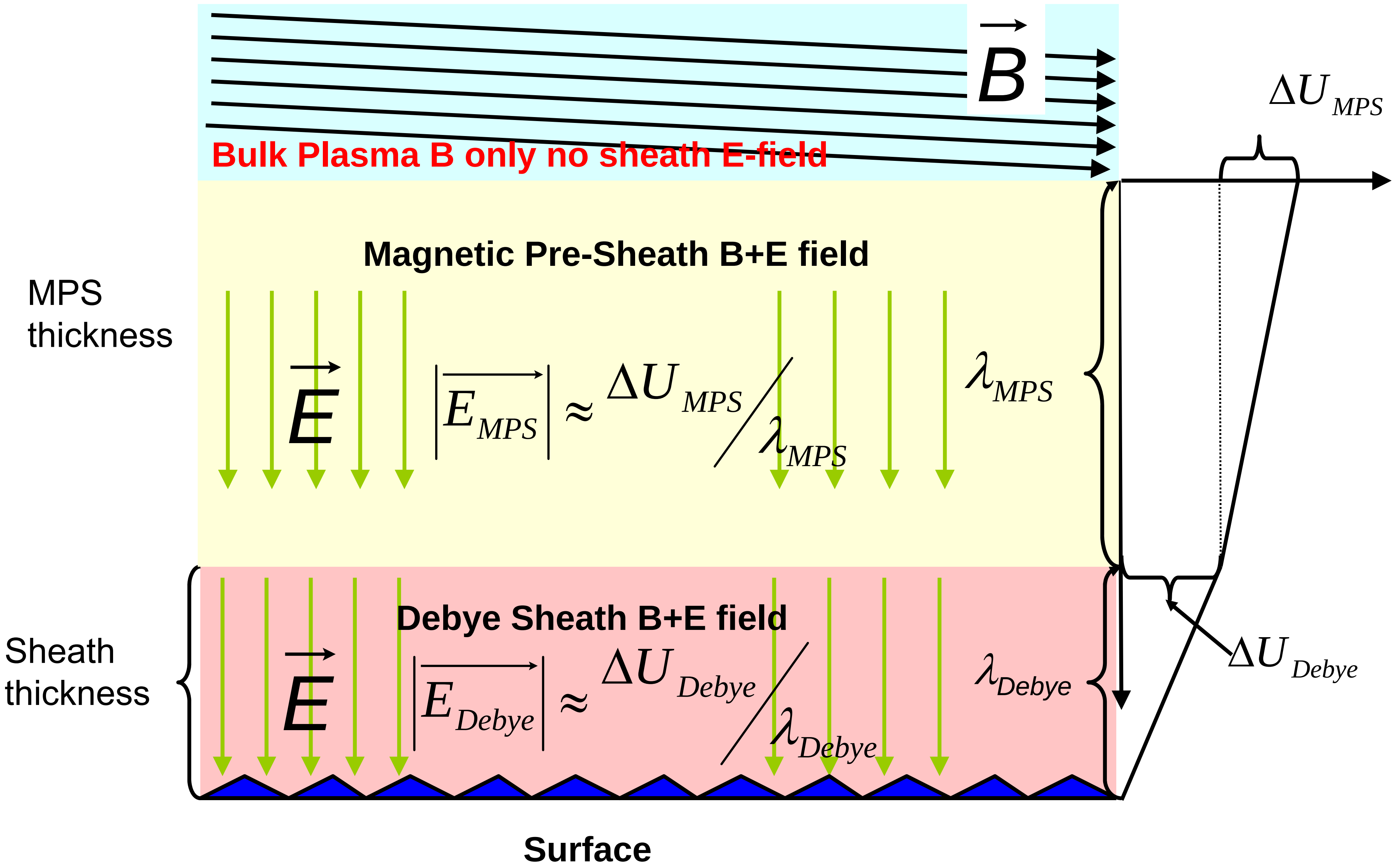
Modeling particle trajectories in the sheath

- To calculate erosion fluxes one needs:
  - Energy & Impact angles of energetic ions incident from the plasma
    - Calculate trajectories and surface impact of particles moving in the sheath region of the plasma
      - Model the electric fields in the sheath region
      - Solve the equations of motion of particles in the sheath region

- **Details see:** ***K. Schmid et. Al Nucl. Fusion 50 (2010) 105004***

Modeling particle trajectories in the sheath

➢ *Approximating the E-fields in the sheath*



❖With respect to initial conditions two cases are distinguished:

1. "Long range transport particles"

    ➢Enter the sheath region from the bulk plasma on gyro orbits

2. "Prompt re-deposited particles"

    ➢Are sputtered and emitted with a cosine distribution

    ➢Are ionized either within their gyro orbit radius or inside the MPS

Impact angle distributions

❖Input parameters used in calculation

Parameter	B (T)	δ (°)	T_e (eV)	n_e (m^{-3})	$\frac{v_{\|\|}}{c_s}$
Central value	1	5	20	10^{18}	1
Variation range	0.5-2	4-10	$10 - 30$	$10^{18} - 10^{19}$	0.1 - 1

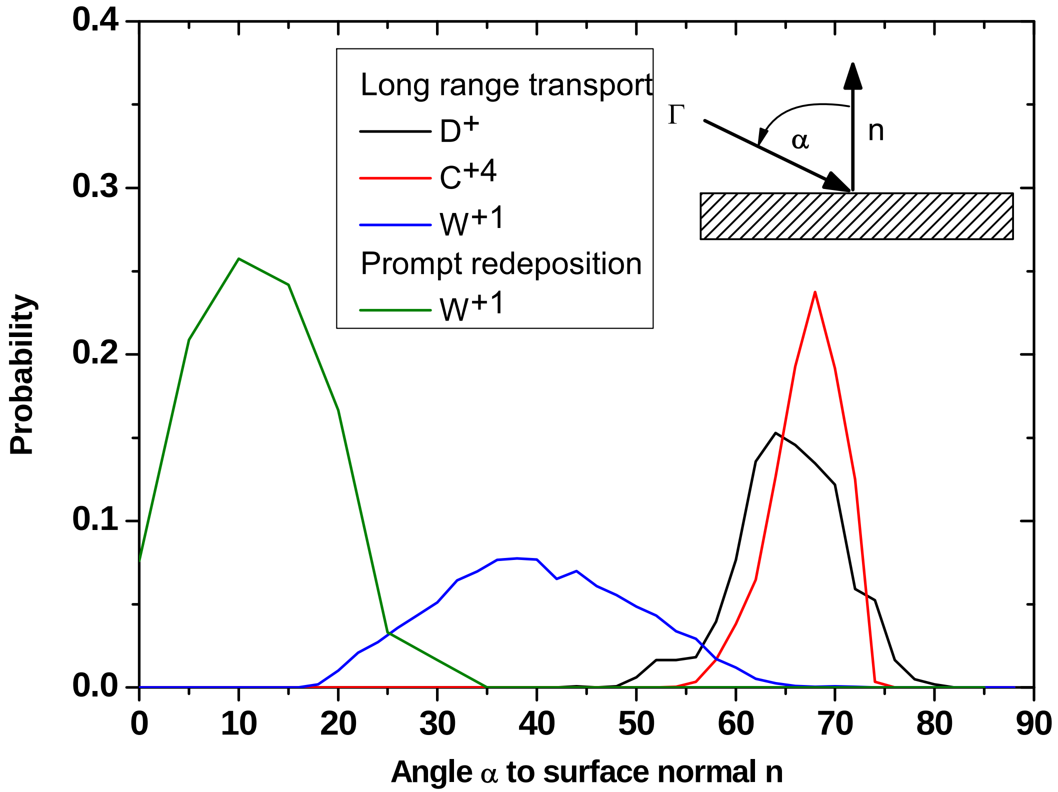
- l_{MPS}~ 2000 μm
- l_{Debye}~ 33μm
- E_{MPS} ~ $2x10^4$ V/m
- E_{Debye} ~ $2x10^5$ V/m

Impact angle distributions

❖ (E+B Field)

•Long range transport: Sample Ω, and Maxwell distribution

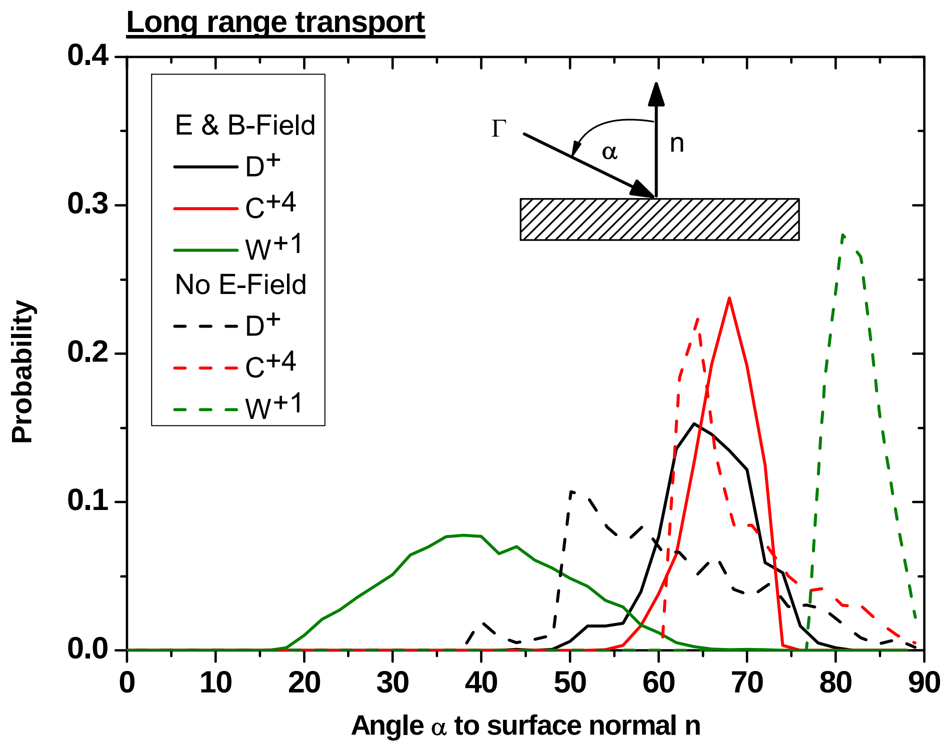
•For prompt redep.: Sample cosine distribution and ionization distance

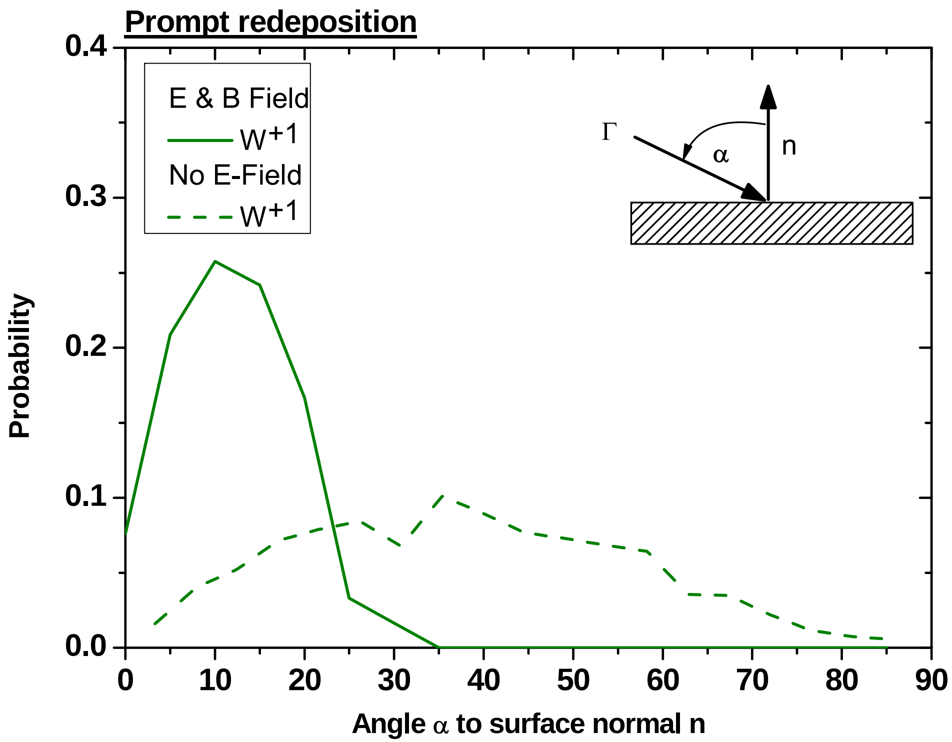


➢Long range transport particles impact at oblique angles

➢Prompt re-deposited particles impact along surface normal

❖ (B Field only)





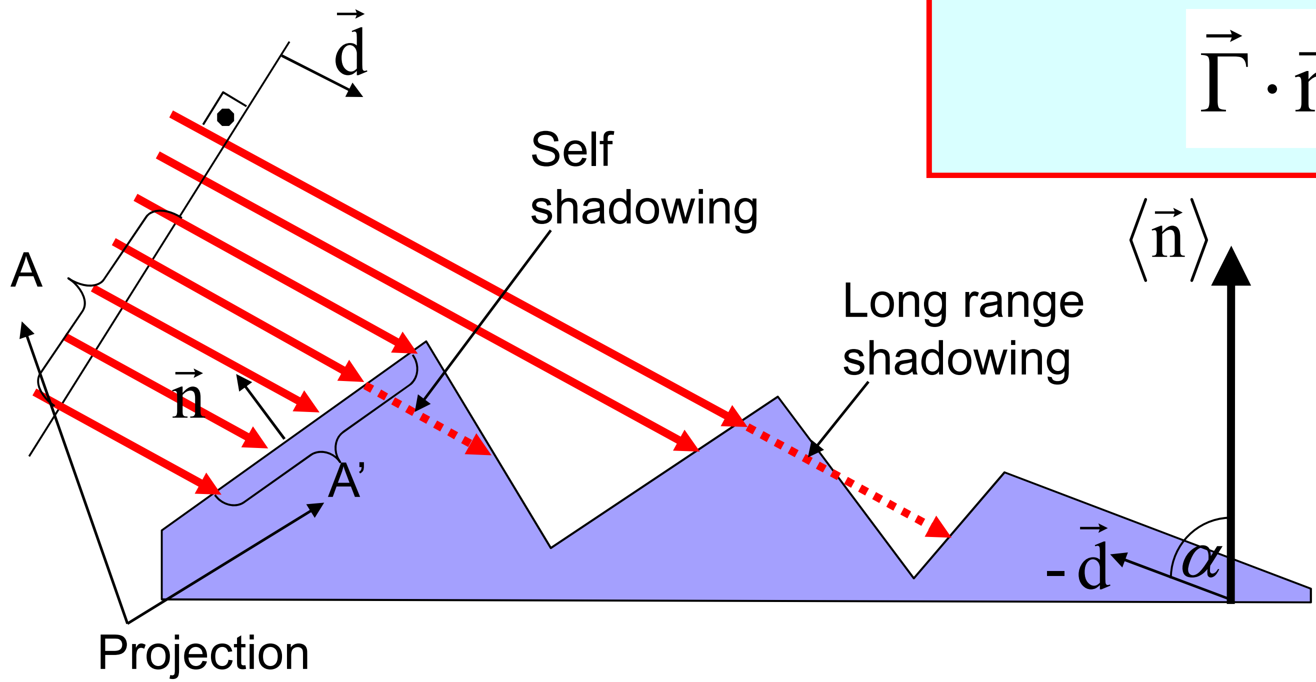
- ➢Sheath acceleration has strongest influence on slow, heavy (q/m << 1) ions
- ➢Prompt re-deposited particles are effected most

Variation of flux across rough surfaces

❖Flux distribution of particles incident at angle α with respect to average surface normal

→ Lateral variation of flux & erosion determined by variation in

$$\vec{\Gamma}\cdot\vec{n}\,(x,y)$$



$$\Gamma(x,y)=\Gamma_0\, f_{Proj}(x,y)\, f_{Self-shadow}(x,y) f_{Long\ range\ shadow}(x,y)$$

Variation of flux across rough surfaces

→ Possible explanation for experimentally observed erosion / deposition patterns

❖Erosion on leading edged due to “Long range transport particles”

➢Oblique impact angles are ~affected by roughness

❖Homogeneous deposition due to “Prompt re-deposited particles”

➢Normal impact angles are ~**un**affected by roughness

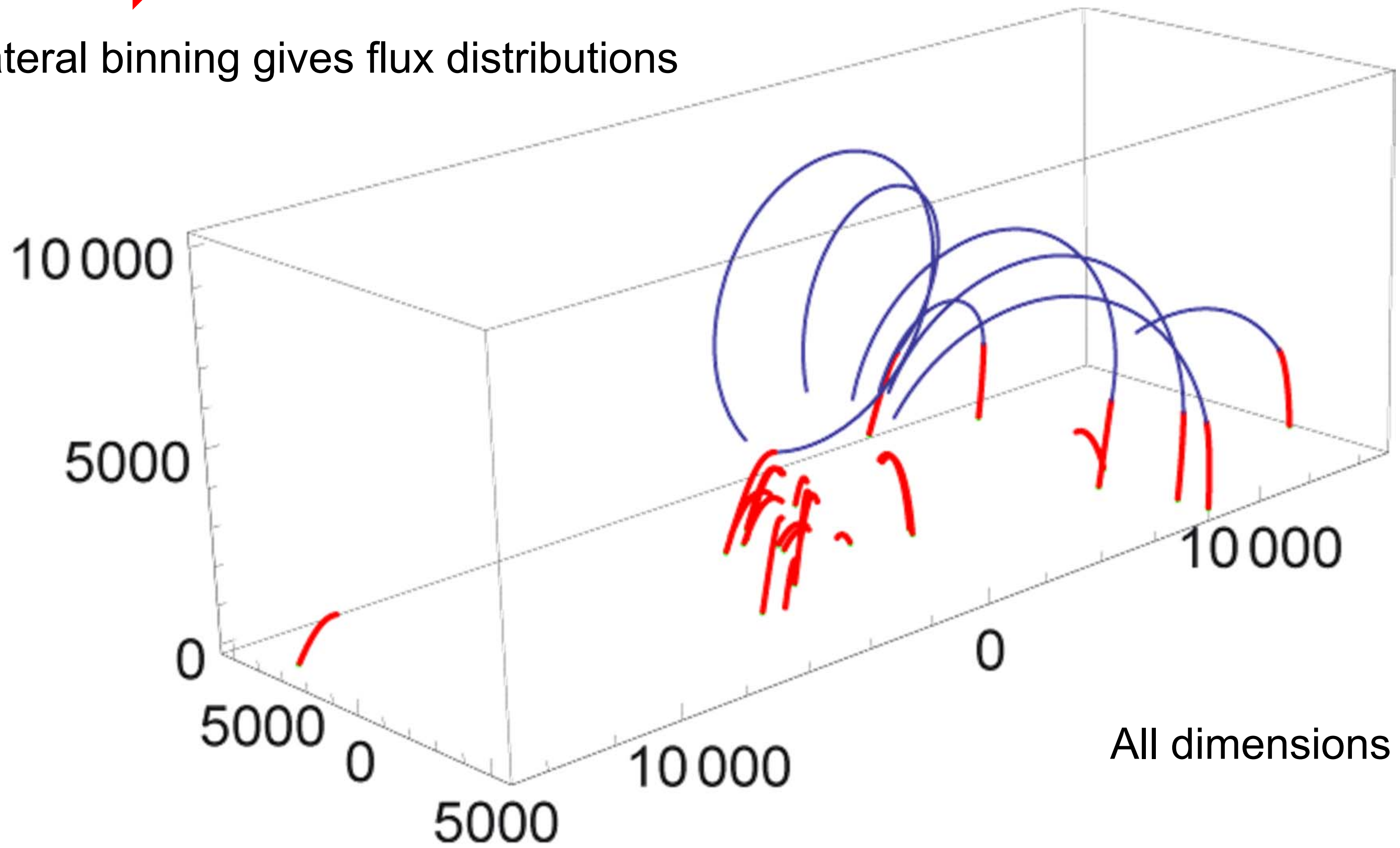
To test hypothesis→ Calculate flux distributions on real surfaces

Flux distributions on real surfaces

❖Ray tracing of particles, sampling the potential range of initial conditions
❖Calculate first impact of trajectory with rough surface

→ $\vec{v}_{Impact}, \vec{r}_{Impact}$

❖Lateral binning gives flux distributions



All dimensions in μm

Flux distributions on real surfaces

❖Calculate erosion depth due to D and C^{+4} impact including

❖Prompt re-deposition of W
❖W self-sputtering

•Net erosion flux on bin j:

$$\Gamma^{ERO}_{net,j} = \left(\Gamma^{ERO,byD}_{j}(1-\nu_c)\right) + \left(\Gamma^{ERO,byC}_{j}(\nu_c)\right) + \Gamma^{ERO}_{net,j} * R * Y_j^{\text{Eff by W}} - (\Gamma^{ERO}_{net,j} * R(1-\text{Refl})) \quad (20)$$

$\Gamma^{ERO,byD}_{j}, \Gamma^{ERO,byC}_{j}$ = Erosion flux due to impact of D and C^{+4} respectively

ν_c = Fraction of C^{+4} in the incident flux

R = Fraction of eroded W that is prompt re-deposited

$Y_j^{\text{Eff by W}}$ = Effective W self sputtering yield due to prompt re-deposited W at bin j

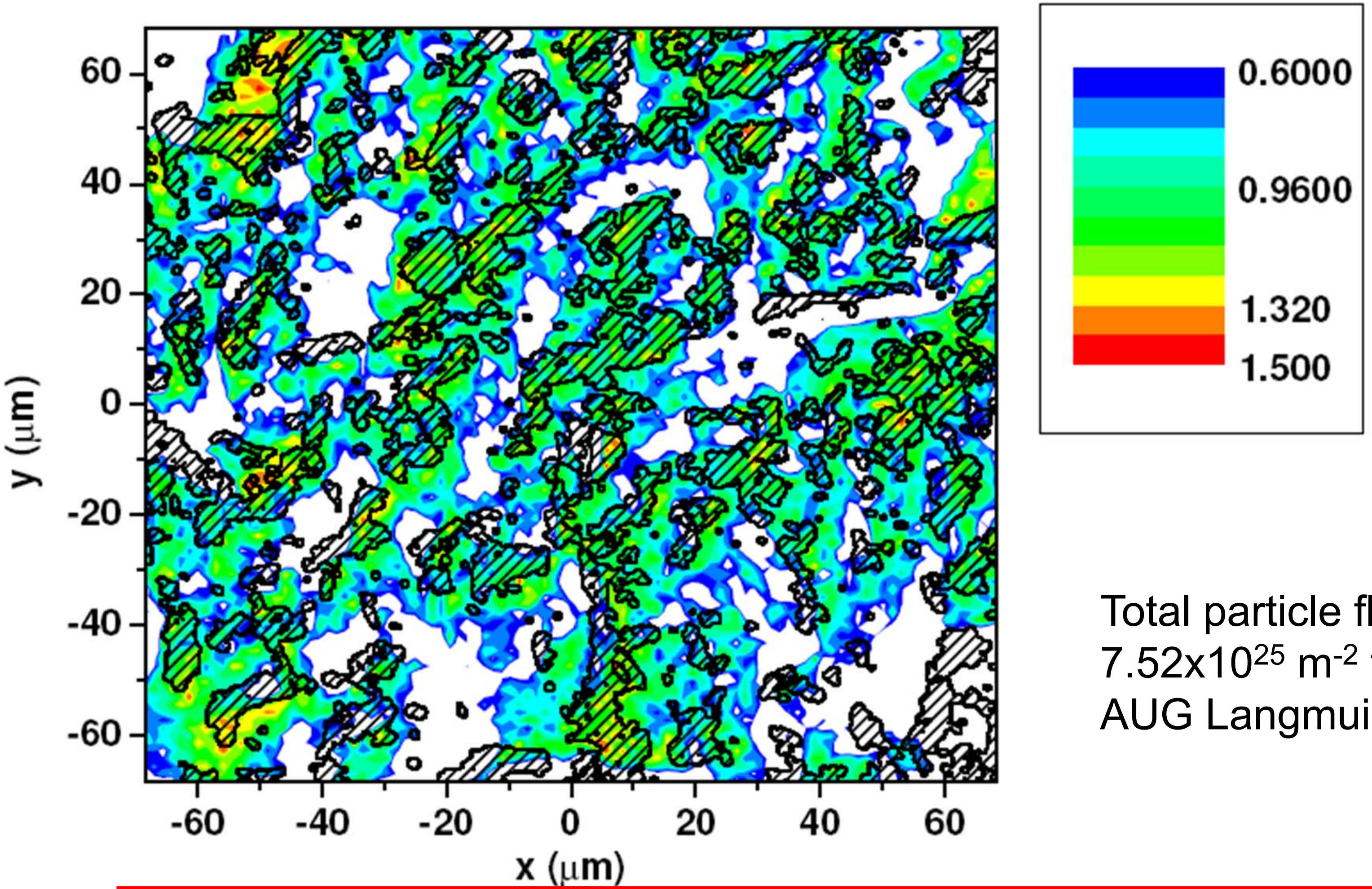
Refl = W reflection yield

➢Solve equation 20 for $\Gamma^{ERO}_{net,j}$ multiply with time and divide by W number density

→ Total erosion depth

Flux distributions on real surfaces

❖Calculated erosion depth for ν_c = 0.3% and R = 30%



Total particle fluence of 7.52×10^{25} m^{-2} taken for AUG Langmuir probe data

➢Calculated erosion pattern matches experimental erosion patterns using reasonable values for ν_c and R

Conclusions

- A model explaining inhomogeneous erosion deposition on rough surfaces based on ExB motion in the plasma sheath is proposed:
  - Long range transport particles erode the leading edges
  - Prompt re-deposited material deposits homogeneously, also areas shadowed to the long range transport particles
- The acceleration in the electrostatic sheath field has a strong impact on the impact angle distribution. (In particular for heavy ions)
- The model reproduces both the erosion pattern shape and the total amount of eroded material.

Discussion slides

Modeling particle trajectories in the sheath

➢*Approximating the E-fields in the sheath*

$$\Delta U_S = \frac{1}{2} T_e \log\left(\frac{2\pi m_e (T_e + T_i)}{T_e m_i}\right)$$

T_i, T_e = Ion and electron temperature respectively

m_i, m_e = Ion and electron mass respectively

❖Total sheath potential drop

❖~constant with B-field angle δ

$$\Delta U_S = \Delta U_{MPS} + \Delta U_{DS}$$

MPS = Magnetic pre-sheath, DS = Debye sheath

$$\Delta U_{MPS} = \frac{T_e}{e_0} \ln\left(\cos(\pi - \delta)\right)$$

$$l_{MPS} = \sqrt{6}\left(\frac{c_s}{\omega}\right)\sin(\delta)$$

$$E_{MPS} = \frac{\Delta U_{MPS}}{l_{MPS}}$$

❖MPS part of the total sheath drop

❖Varies with B-field angle δ

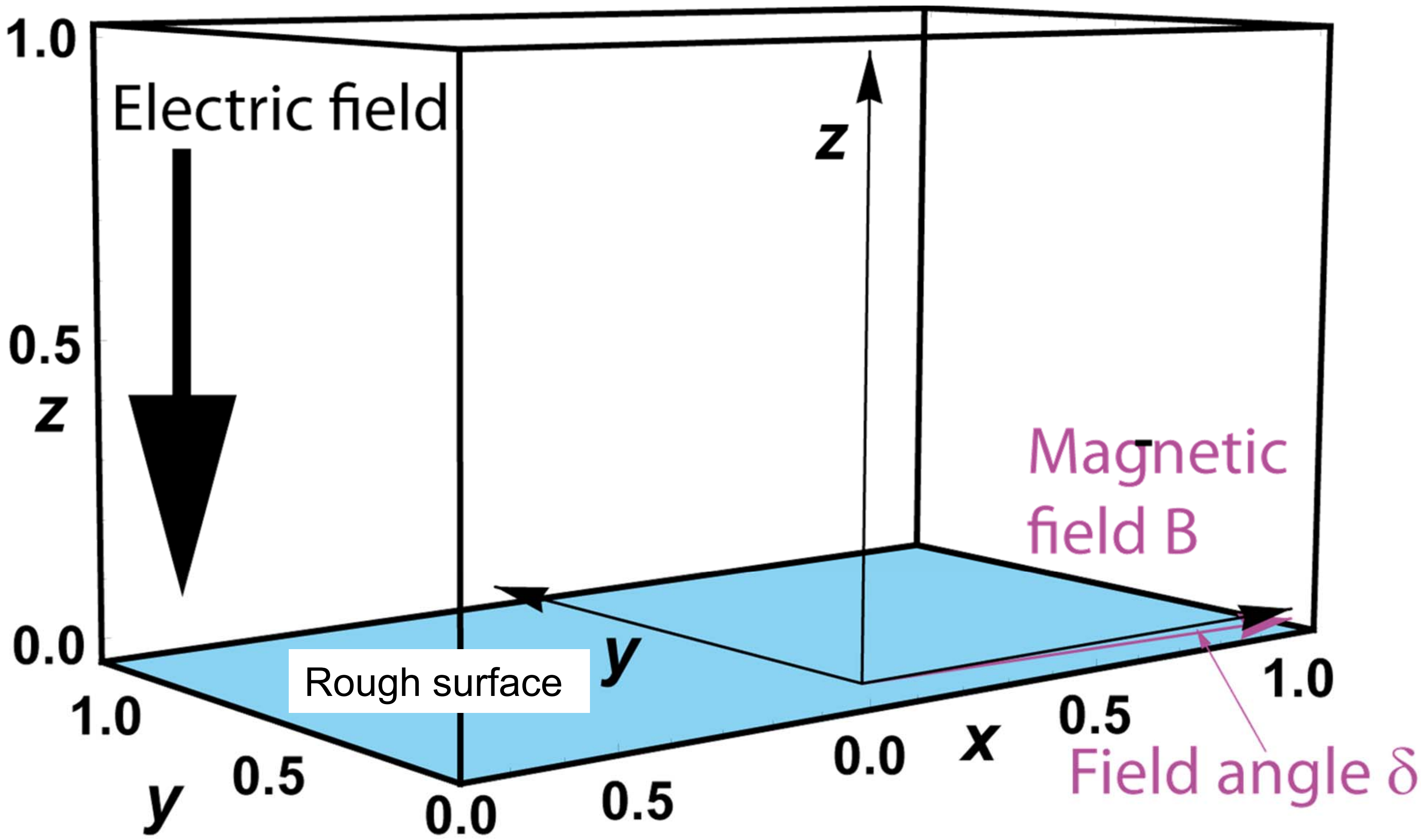
$$\Delta U_{DS} = \Delta U_S - \Delta U_{MPS}$$

$$l_{DS} = \sqrt{\frac{\epsilon_0 T_e}{e_0 n_e}}$$

$$E_{DS} = \frac{\Delta U_{DS}}{l_{DS}}$$

❖Debye part of the total sheath drop

❖Coordinate system used



Modeling particle trajectories in the sheath

➢ *Solving the equations of motion*

❖ Equations of motion

$$
\begin{aligned}
\ddot{x}(t) &= \beta B_Z \dot{y}(t) \\
\ddot{y}(t) &= \beta \left(B_X \dot{z}(t) - B_Z \dot{x}(t) \right) \\
\ddot{z}(t) &= \beta \left(-B_X \dot{y}(t) - E_Z \right) \\
\beta &= \frac{q}{m} \text{ Charge to mass ratio} \\
E_Z &= \text{Z-Component of the electrical field } \vec{E} = (0, 0, E_Z)
\end{aligned}
$$

➢ Solved using Mathematica, yields analytical solution

➢ Trajectories require initial conditions: $\vec{r}(t=0) = \vec{r}_{\mathrm{Init}}$

$$\dot{\vec{r}}(t=0) = \vec{v}_{\mathrm{Init}}$$

Modeling particle trajectories in the sheath

➢*Solving the equations of motion*

1. "Long range transport particles"

δ = magn. Field angle

$$\vec{v}_{init} = (v_{||}, V_{\perp}, 0) \cdot \mathbf{M}$$

$$\mathbf{M} = \mathbf{R}(\Omega, (1,0,0)) \cdot \mathbf{R}(\delta, (0,1,0))$$

$$v_{||} = \text{Velocity along magnetic field}$$

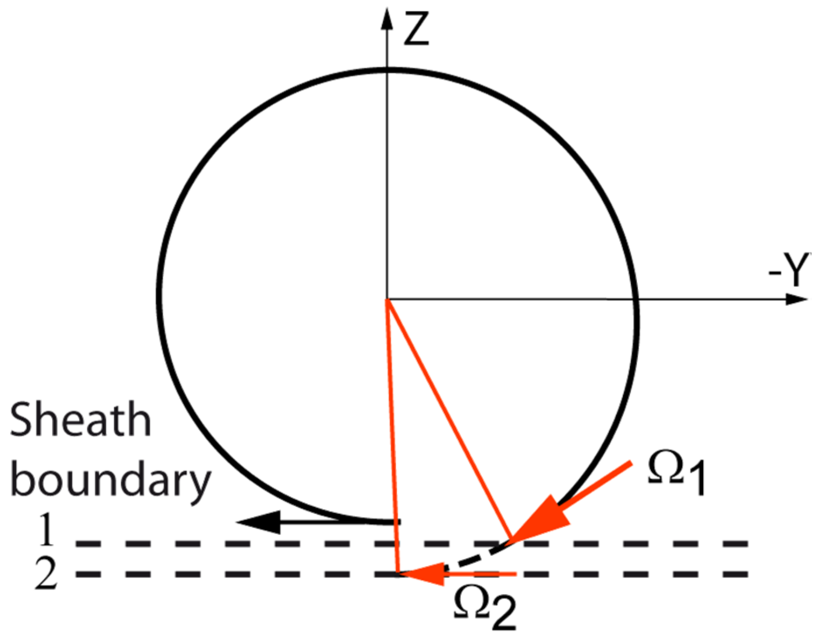
$$v_{\perp} = \text{Velocity perpendicular to magnetic field}$$

Ω = Gyro orbit phase angle on MPS impact

➢Ω Depends on velocity $v_{II}/v_{\perp}$ and q/m ratio

$$|v_{||}| \sim v_{\text{Bohm-D}}(T_e)$$

$$|v_{\perp}| \sim \text{Maxwell distributed}(T_e)$$

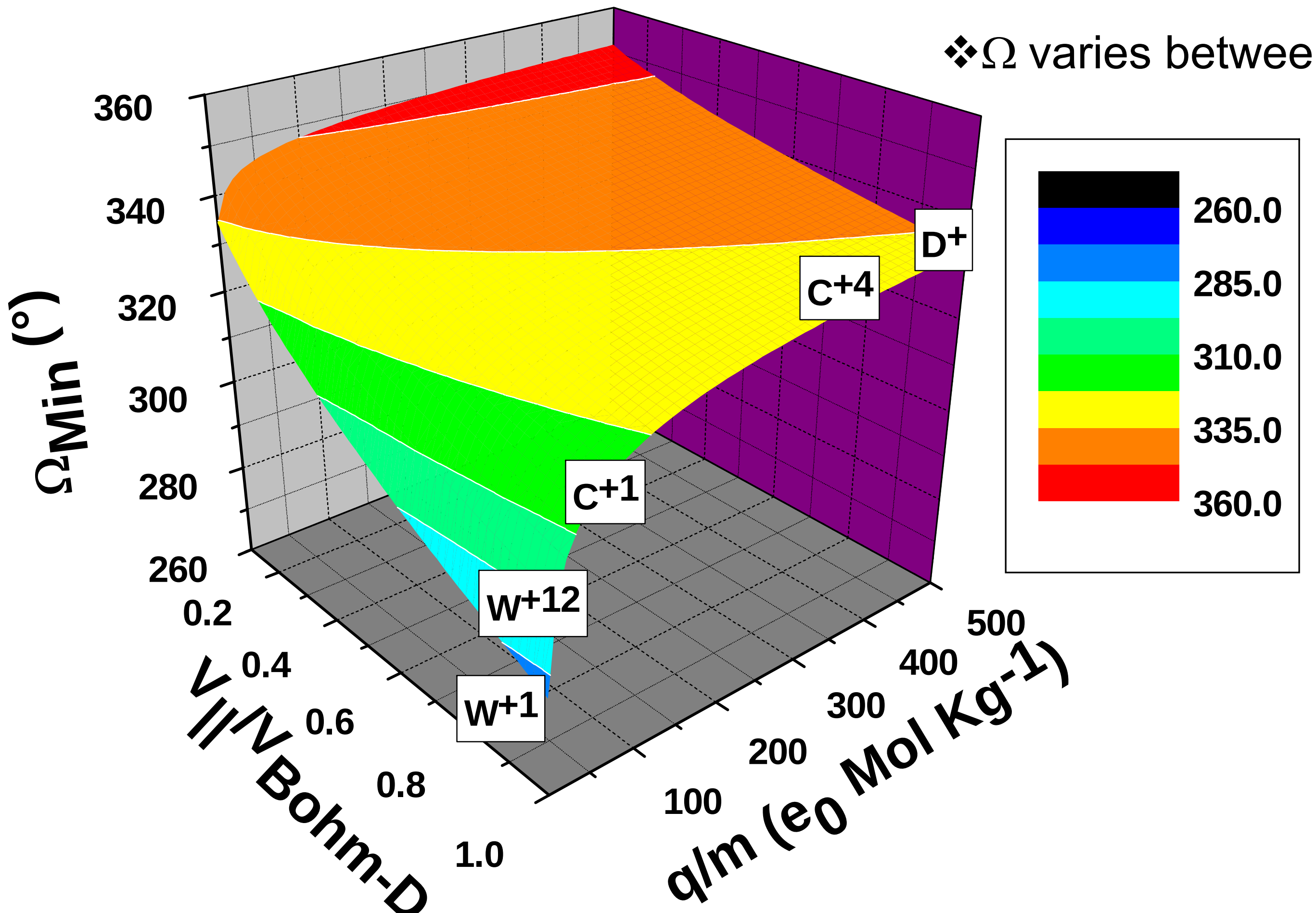


Modeling particle trajectories in the sheath

➢*Solving the equations of motion*

❖Possible values for Ω for "Long range transport particles"

❖Ω varies between Ω_{Min} and Ω_{Max}=360°



➢Light particles→ Small impact angle range→Narrow impact angle distribution
➢Heavy particle→Broad impact angle range→ Broad impact angle distribution

2. “Prompt re-deposited particles”

❖“Sputter launch” according to cosine distribution

$$\begin{aligned}\vec{d}_{Cos} &= (0,0,1)\cdot\mathbf{R}(\vartheta,(1,0,0))\cdot\mathbf{R}(\varphi,(0,0,1))\\ \vartheta &= \arcsin\left(\sqrt{r_\vartheta}\right)\\ \varphi &= 2\pi r_\varphi\\ \mathbf{R}(\alpha,\vec{r}) &= \text{Rotation matrix around axis } \vec{r} \text{ by angle } \alpha\\ r_\varphi, r_\vartheta &= \text{Uniform random numbers from 0-1}\end{aligned}$$

$\vec{V}_{Init}$

❖Initial velocity ½ surface binding energy (typical for physical sputtering)

$$\begin{aligned}|\vec{v}_{init}| &= \sqrt{\frac{2\langle E_{Sput}\rangle}{m}}\\ \langle E_{Sput}\rangle &= \text{Mean energy of sputtered particles}\\ m &= \text{Mass of sputtered particle}\end{aligned}$$

Modeling particle trajectories in the sheath

➢ *Solving the equations of motion*

2. “Prompt re-deposited particles”

❖ Ionized to +1 at normal distance z above surface

$$z_{\mathrm{Min}} < z < z_{\mathrm{Max}}$$

$$z_{\mathrm{Min}} = \lambda_{\mathrm{Debye}}$$

$$z_{\mathrm{Max}} = \max(l_{\mathrm{MPS}}, r_{\mathrm{gyro}})$$

→ For W^{+1} typical ionization distance from surface is several mm

❖ No variation in ionization probability within Z_{Min} and Z_{Max} taken into account

- ➢ Feature height ~ Sheath dimension
  - •Surface roughness influences sheath electric field
  - •Requires PIC-Code or similar to calculate field distribution
  - → Can not be treated in the simple frame of this model

- ➢ Feature height >> Sheath dimension
  - •Sheath follows surface roughness
  - •Particles impact locally on "flat" surface
  - •Electric field not homogeneous near edges
  - → Can partly be treated in the simple frame of this model

- ➢ Feature height << Sheath dimension
  - •Sheath not influenced by surface structure
  - •Particles impact along their trajectories on the different surface inclinations
  - → Flux and impact angle distribution can be calculated (see following slides)

Impact angle distributions

❖ Calculate impact angles on flat surfaces

$$\alpha \quad = \arccos\left(\frac{-\vec{v}_{imp} \cdot \vec{n}_{imp}}{|\vec{v}_{imp}| * |\vec{n}_{imp}|}\right)$$

❖Radius of curvature ρ

$$\rho \quad = \frac{|\partial_t \vec{r}(t)|^3}{\partial_t \vec{r}(t) \times \partial_{t,t} \vec{r}(t)}$$ ~ mm >> roughnes

→ Particles impinge essentially along straight lines on the rough surface

Variation of flux across rough surfaces

❖Local surface normal

$$\vec{r} = (x, y, z(x,y))$$
$$\vec{n} = \frac{\partial \vec{r}}{\partial x} \times \frac{\partial \vec{r}}{\partial y}$$

→ **Lateral variation of flux & erosion determined by variation in**

$$\vec{\Gamma} \cdot \vec{n}\,(x, y)$$

❖Projection:

$$\begin{aligned} f_{proj} &= -\vec{\Gamma} \cdot \vec{n} \\ \vec{\Gamma} &= \Gamma_0 * \vec{d} \\ \vec{d} &= \text{Normalized direction vector} \\ \vec{n} &= \text{Local normalized surface normal} \end{aligned}$$

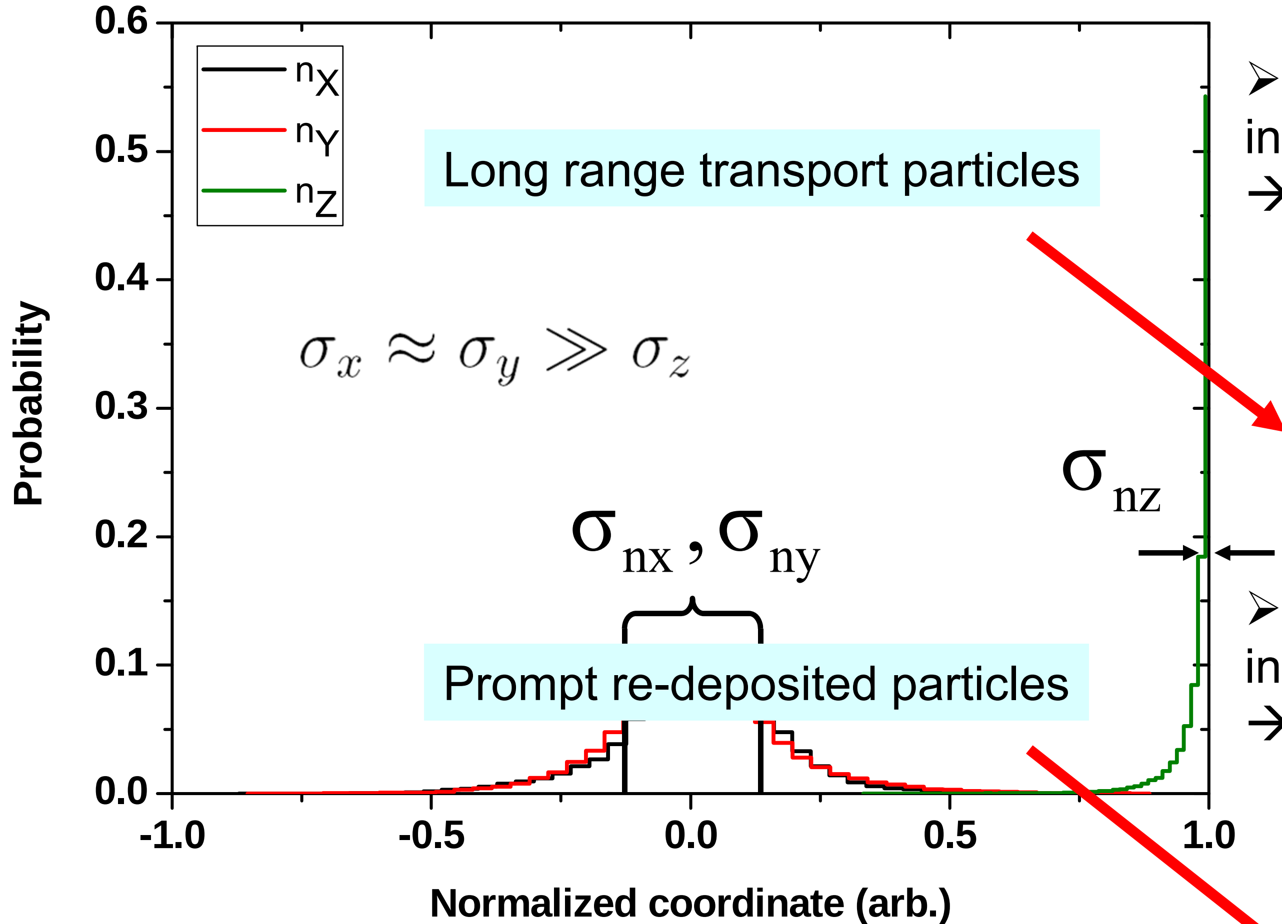
❖Self shadowing:

$$f_{sself} = \begin{cases} 1 & -\vec{\Gamma} \cdot \vec{n} \geq 0 \\ 0 & -\vec{\Gamma} \cdot \vec{n} \leq 0 \end{cases}$$

➢Long range shadowing: Requires ray tracing

Variation of flux across rough surfaces

- Variation in $\vec{\Gamma}\cdot\vec{n}\,(x,y)$ based on σ_{nx}, σ_{ny}, σ_{nz} from gaussian error propagation:



$$\sigma\left(f_{proj}\right) = \sqrt{d_x\sigma_x + d_y\sigma_y + d_z\sigma_z}$$

- Oblique angle of incidence, d_z~0
  → determined by σ_{nx}, σ_{ny}

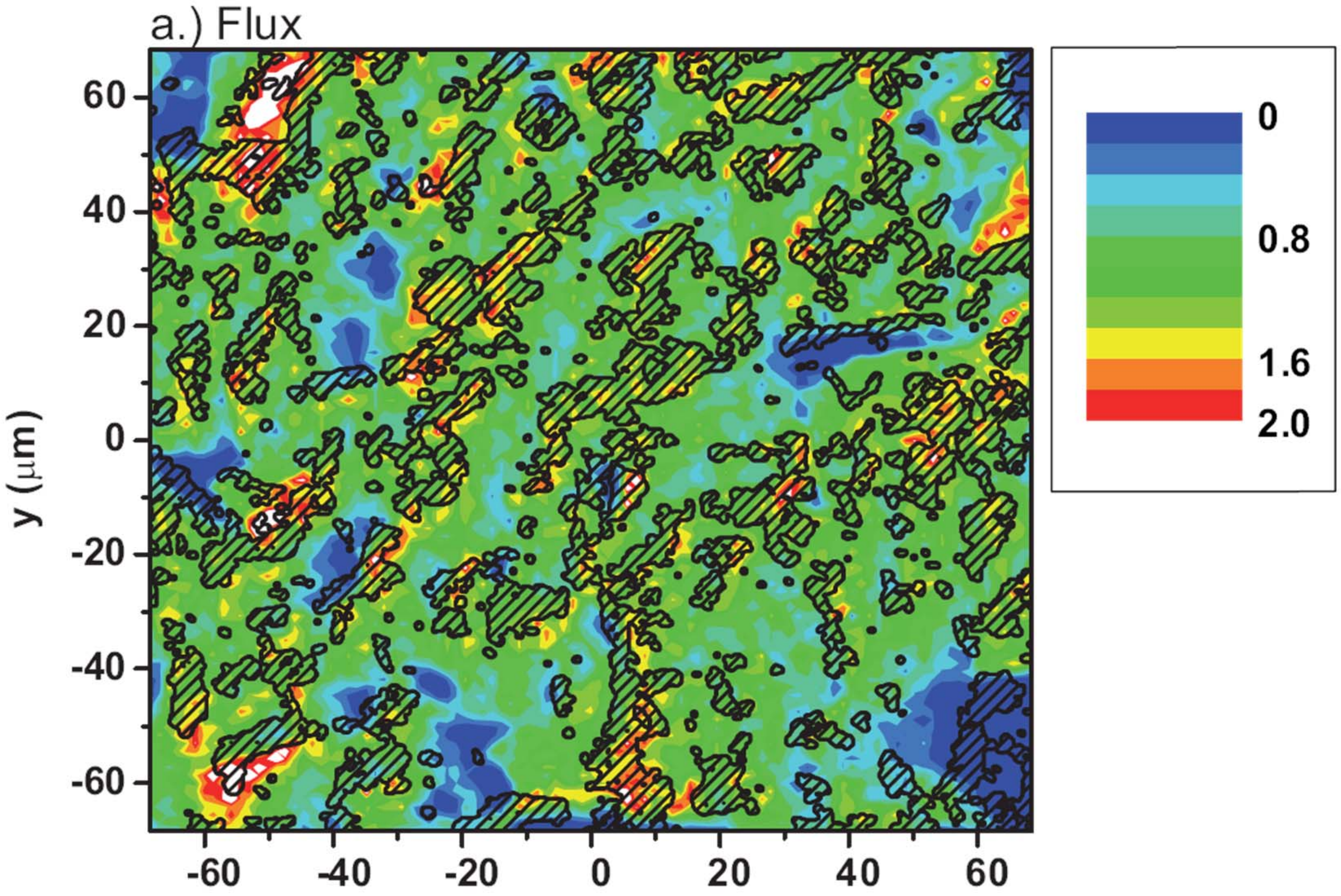
  Broad, **inhomogeneous** distribution

- Normal angle of incidence, d_z~1
  → determined by σ_{nz}

  Narrow, **homogeneous** distribution

Flux distributions on real surfaces

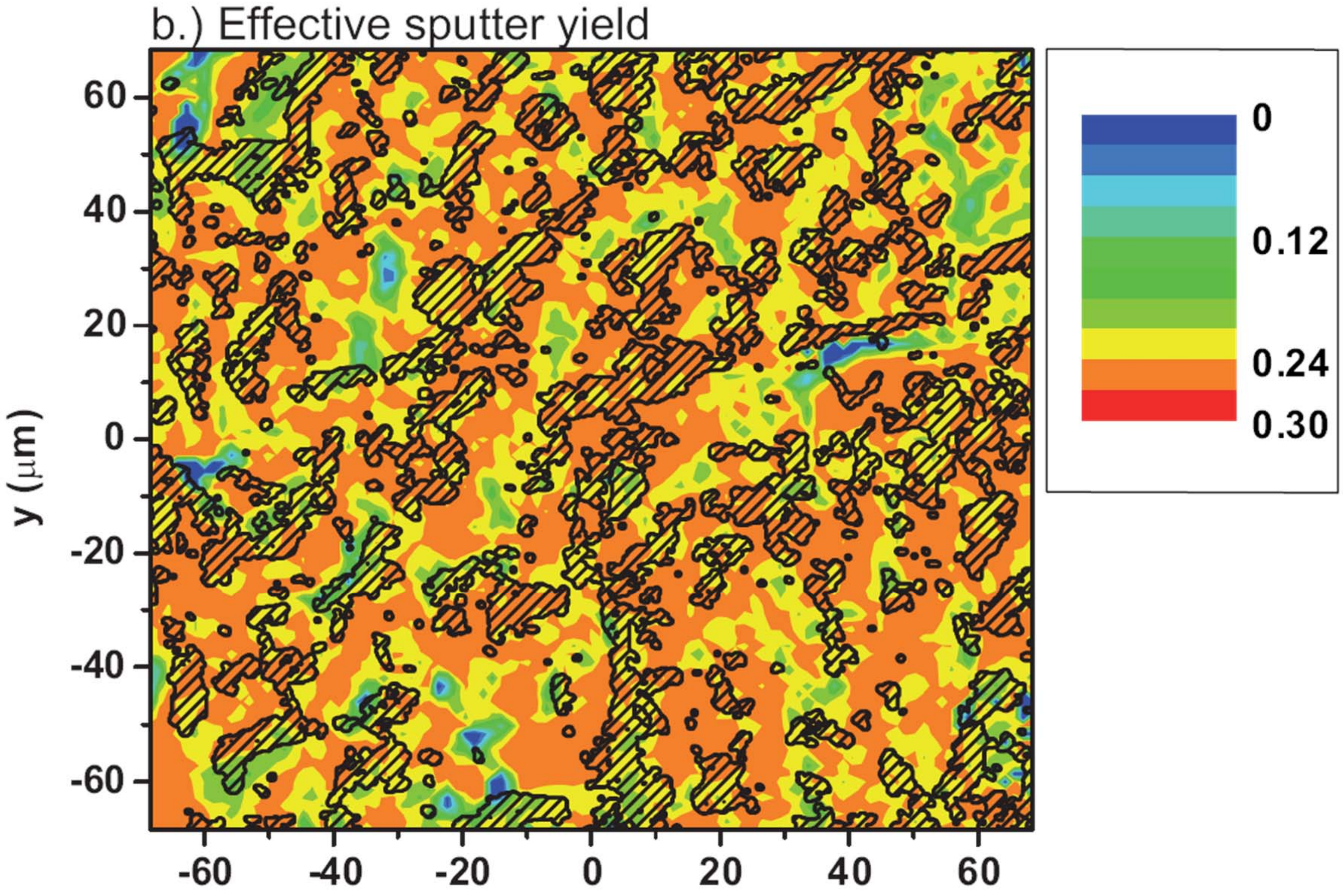
❖Flux distribution of C^{+4} for a total influx of 1 C^{+4} (m^{-2})



➢Flux peaking correlated with experimentally found erosion patterns

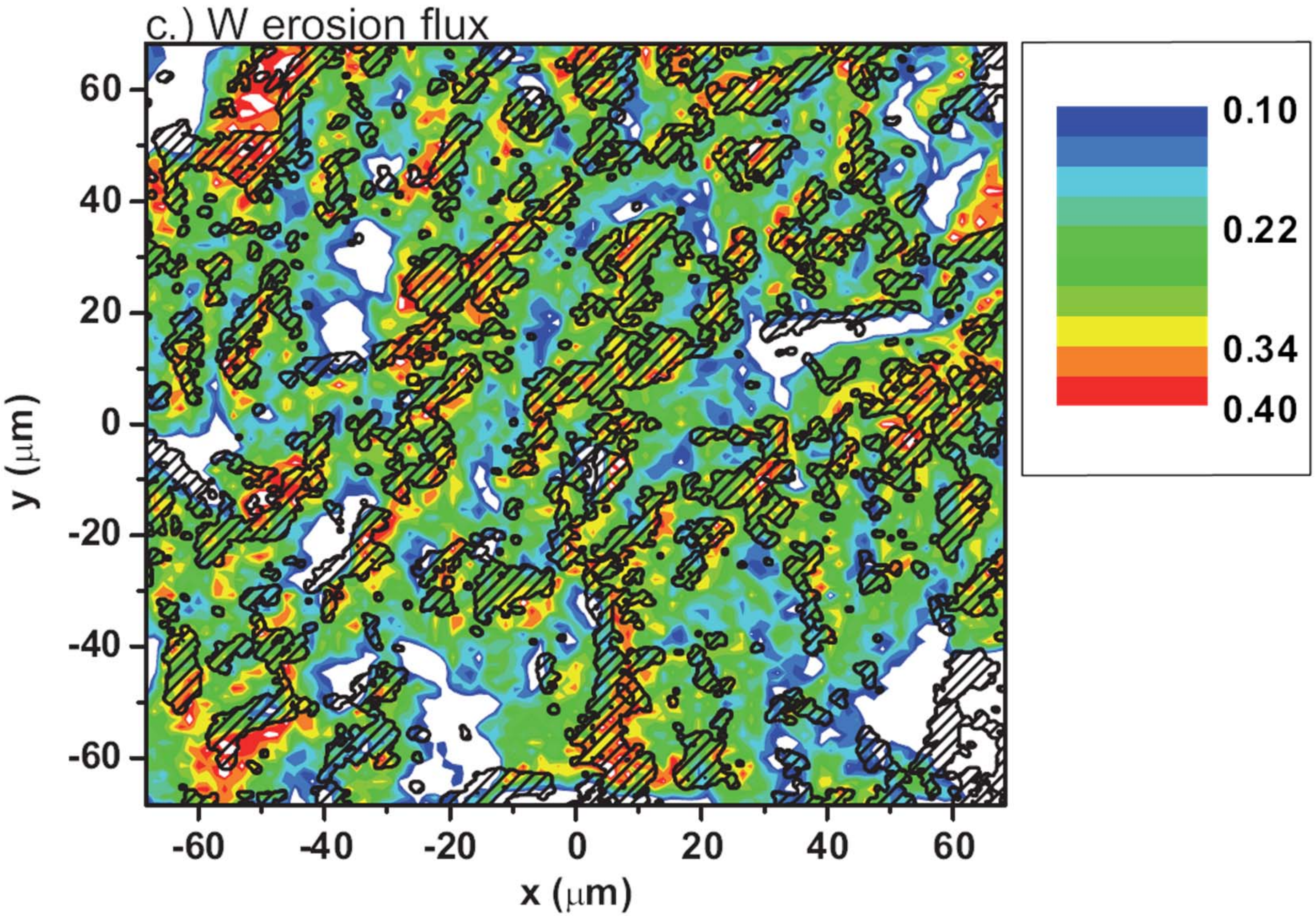
Flux distributions on real surfaces

❖Effective sputter yield of W by C^{+4} using a combination of Bohdansky and Yamamura formula



Flux distributions on real surfaces

❖ W erosion flux by C^{+4} for a total influx of 1 C^{+4} (m^{-2})



➢Areas of peak erosion fit experimentally found erosion patterns