Sputtering of rough and nanostructured W samples

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Jülich 06/02 – 09/02

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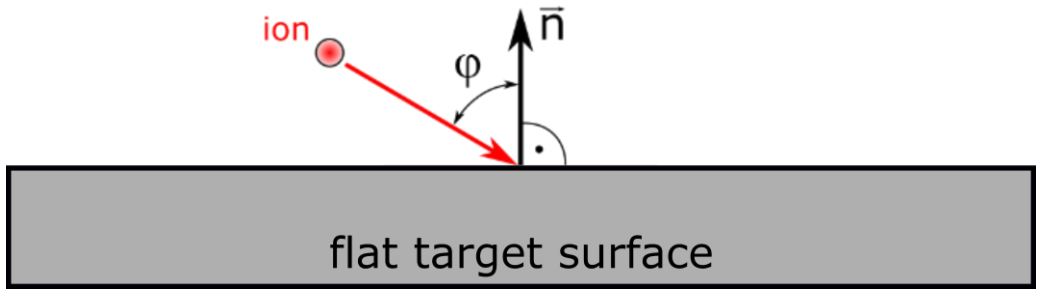
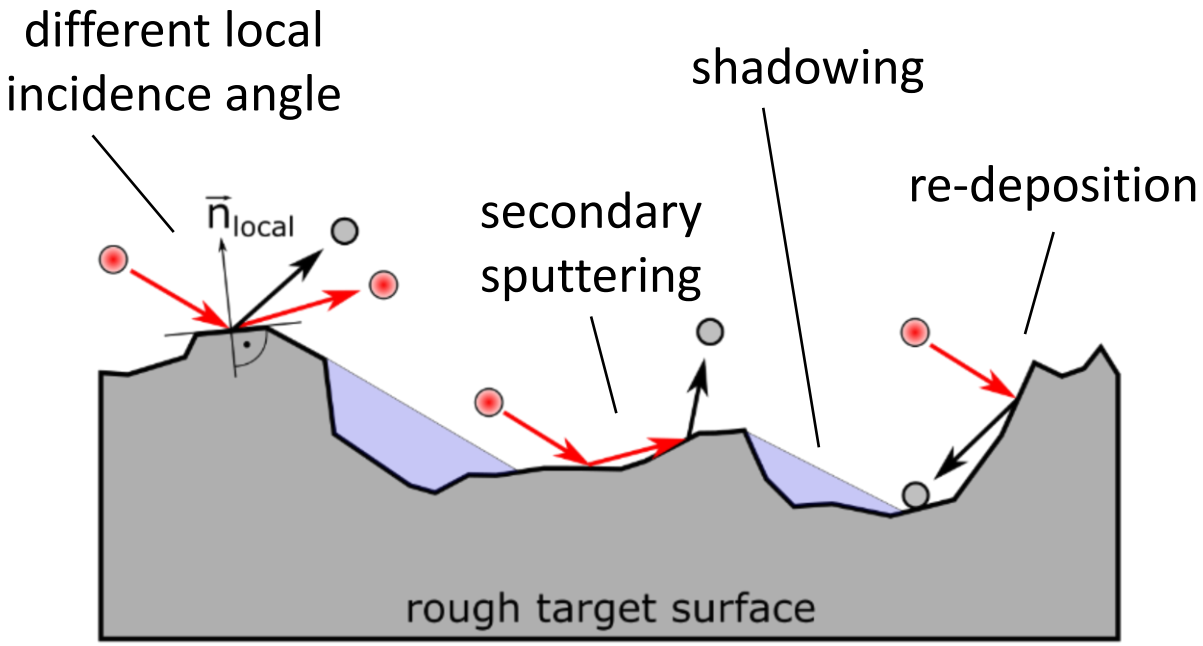
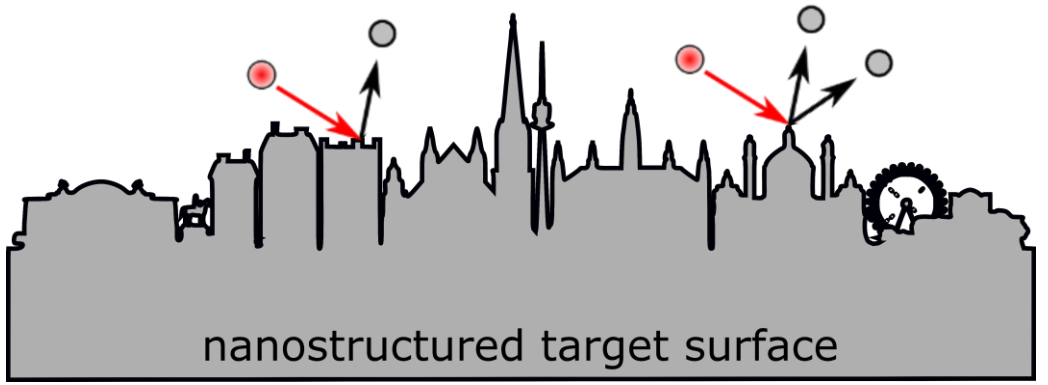






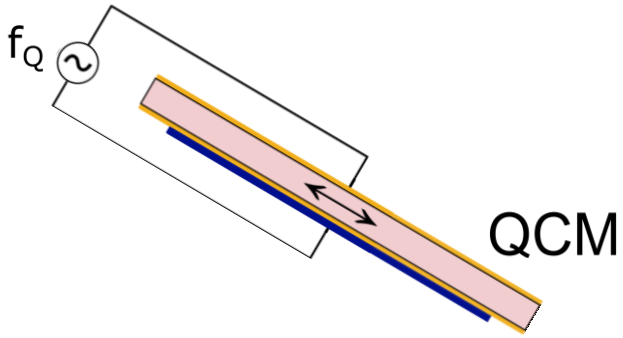
Introduction

Experimental Approach

Simulation Approach

Selected Results and Outlook

Experimental Approach

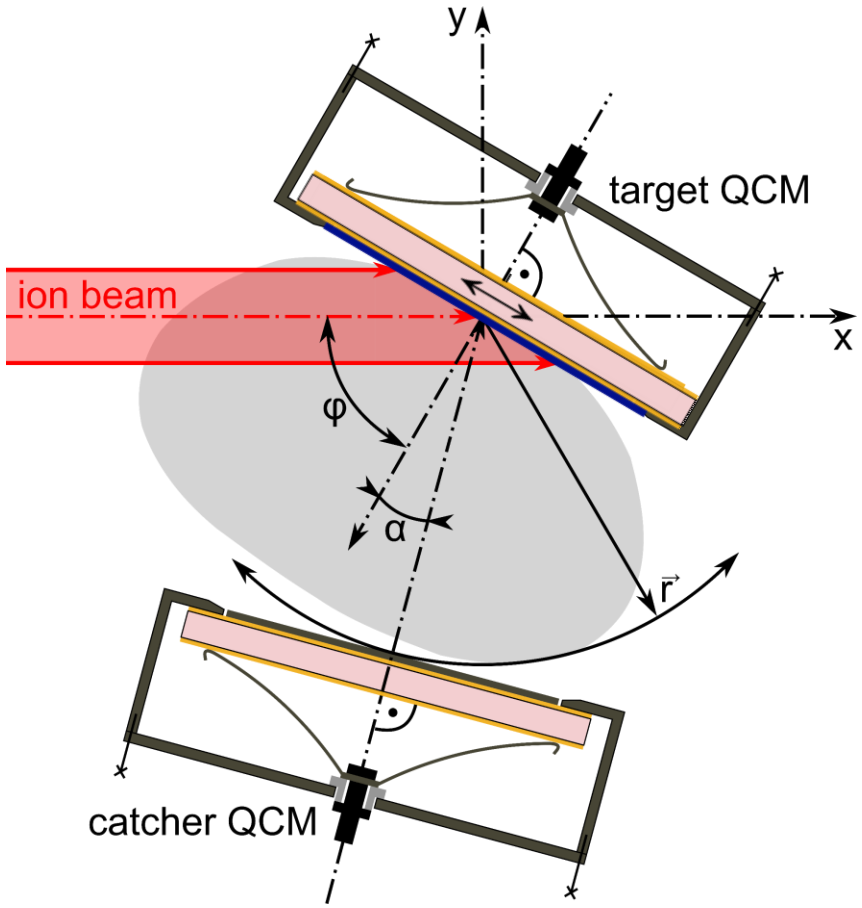


- **Quartz Crystal Microbalance** (QCM) technique: detect mass changes *in-situ*

$$\frac{\Delta f_Q}{f_q} = -\frac{\Delta m_Q}{m_Q}$$

G. Sauerbrey, Zeitschrift f. Physik 155 (1959)

Experimental Approach



- **target erosion** experiments
- probing angular distribution of **sputtered particles**

→ mass change rates down to 10^{-9} g/cm^2/s (~10^{-4} W monolayers/s) can be detected

→ for direct target erosion experiments: thin films deposited on QCM substrate can be investigated

→ for catcher measurements: liberal sample choice possible, sputtered particles are collected with the catcher QCM

G. Hayderer et al., Rev. Sci. Instrum. 70 (1999)
B. M. Berger et al., Nucl. Instrum. Methods. Phys. Res. B 406 (2017)

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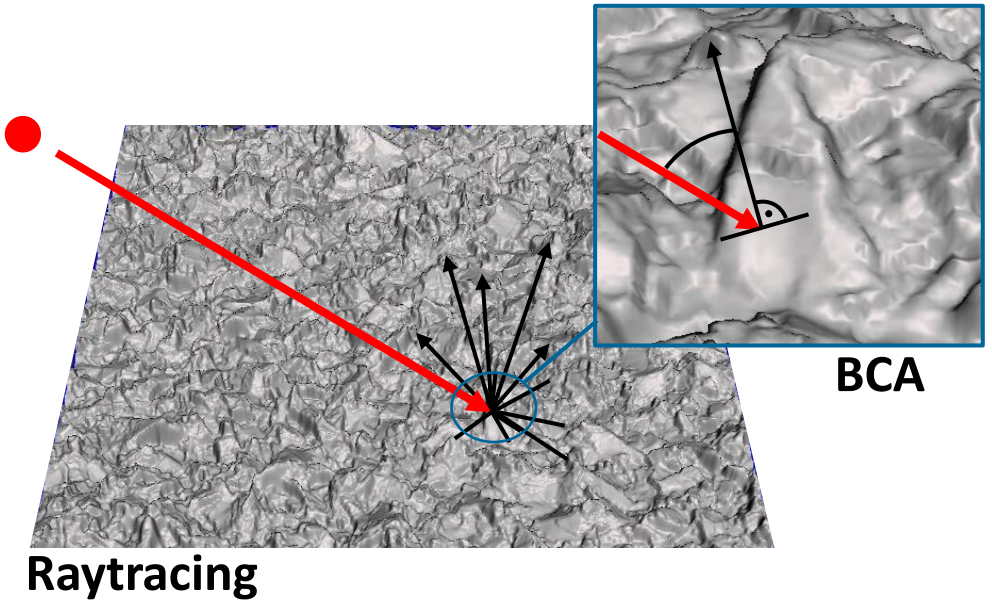
SPRAY = **SP**uttering simulation via **RAY**tracing of particles



→ can be seen as an **add on** for available BCA codes like SDTrimSP

→ utilizes flat **surface repository data from BCA codes**

→ requires a **topography input** (e.g., from qualitative SEM images, quantitative AFM images, artificially generated structures, …)

→ performs a **raytracing loop**

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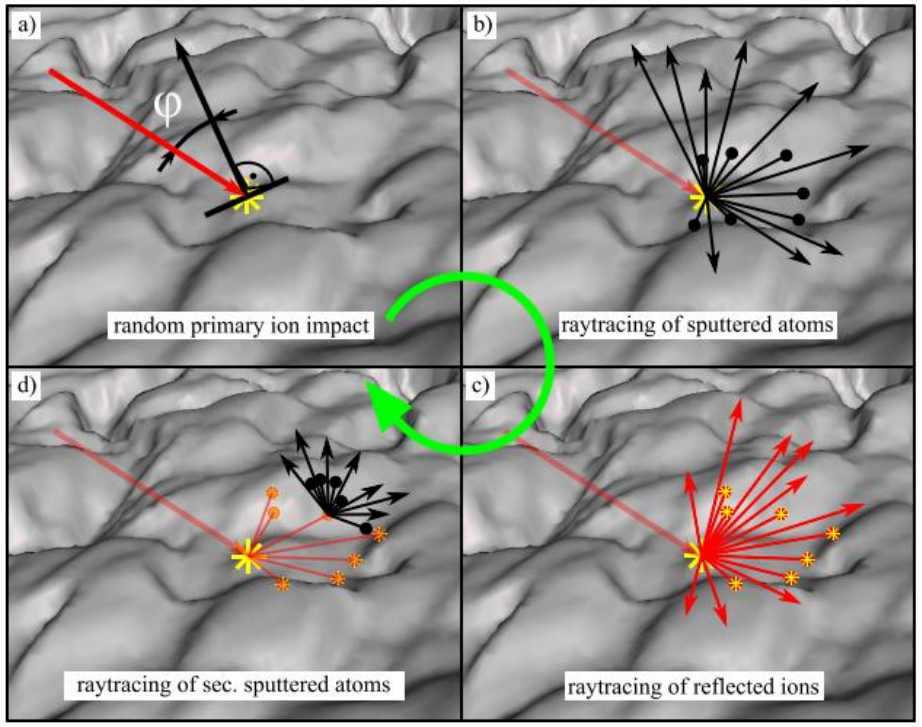

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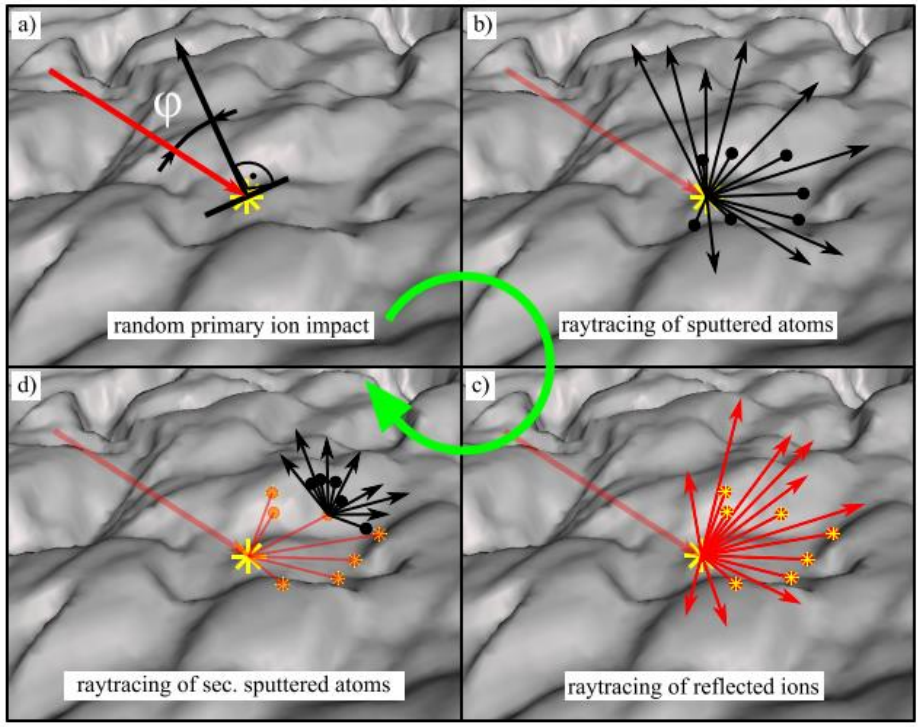


→ performs a **raytracing loop**

a) ion randomly hits the surface – BCA repository

b) sputtered atoms are ejected – redeposition

c) ions get reflected – secondary impact

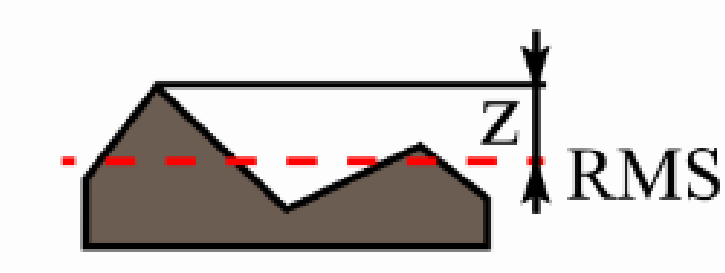
d) secondary sputtering

Simulation Approach

SPRAY = **SP**uttering simulation via **RAY**tracing of particles

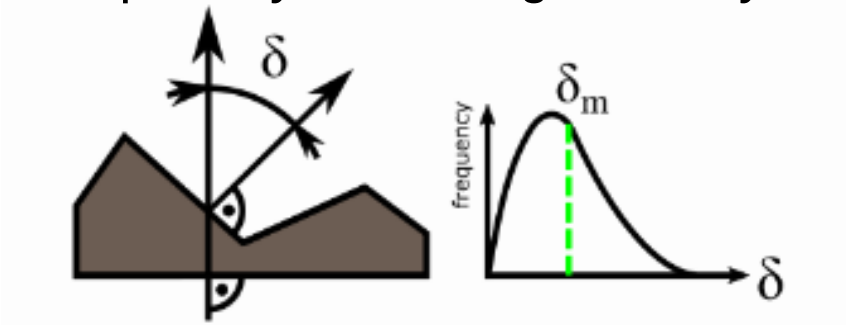
root mean square roughness

→ scale dependent parameter, cannot predict sputter yields



δ_m parameter

→ represents the mean inclination angle, scale independent, can be used to predict sputter yields using an analytical model



C. Cupak et al., Appl. Surf. Sci. 570 (2021)
P. S. Szabo et al., Surf. Interfaces 30 (2022)

Simulation Approach

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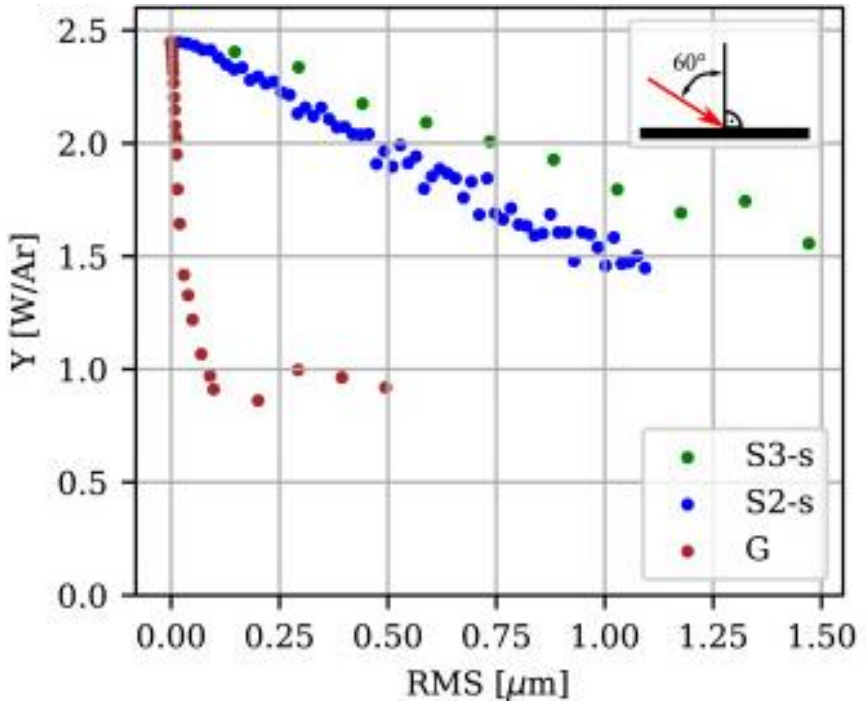
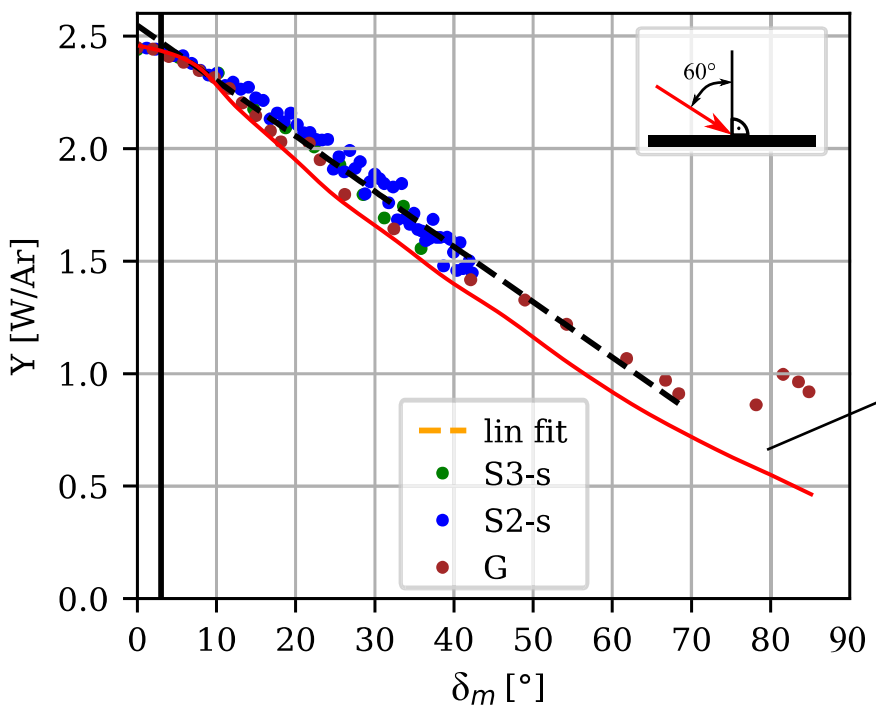


δ_m parameter



analytical model

C. Cupak et al.,
Appl. Surf. Sci. 570 (2021)
P. S. Szabo et al.,
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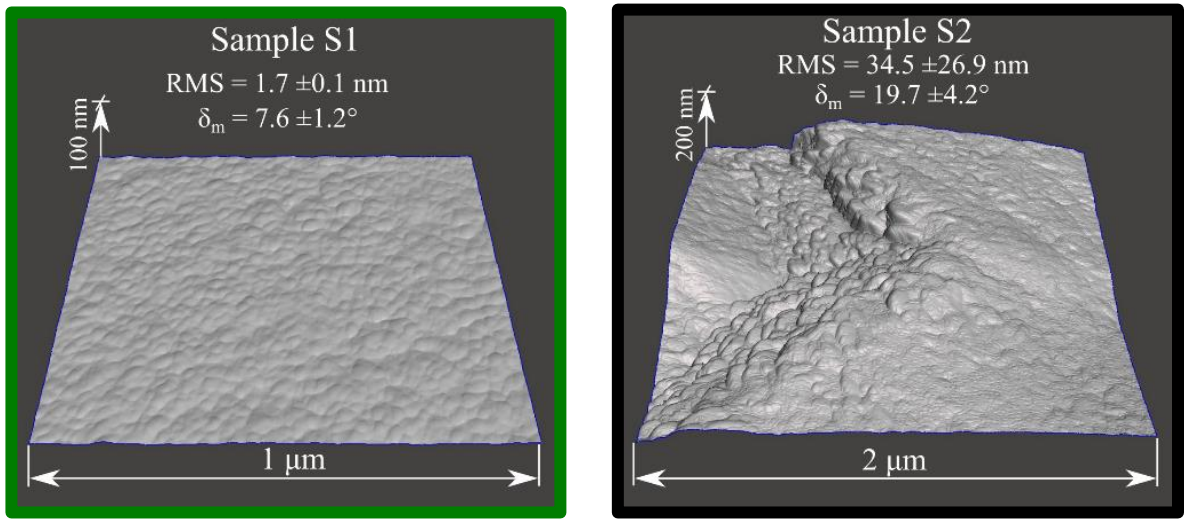
Selected Results and Outlook

Gaussian rough surfaces:



smooth sample **comparably rough sample**

→ sample creation: PVD grown at IPP Garching

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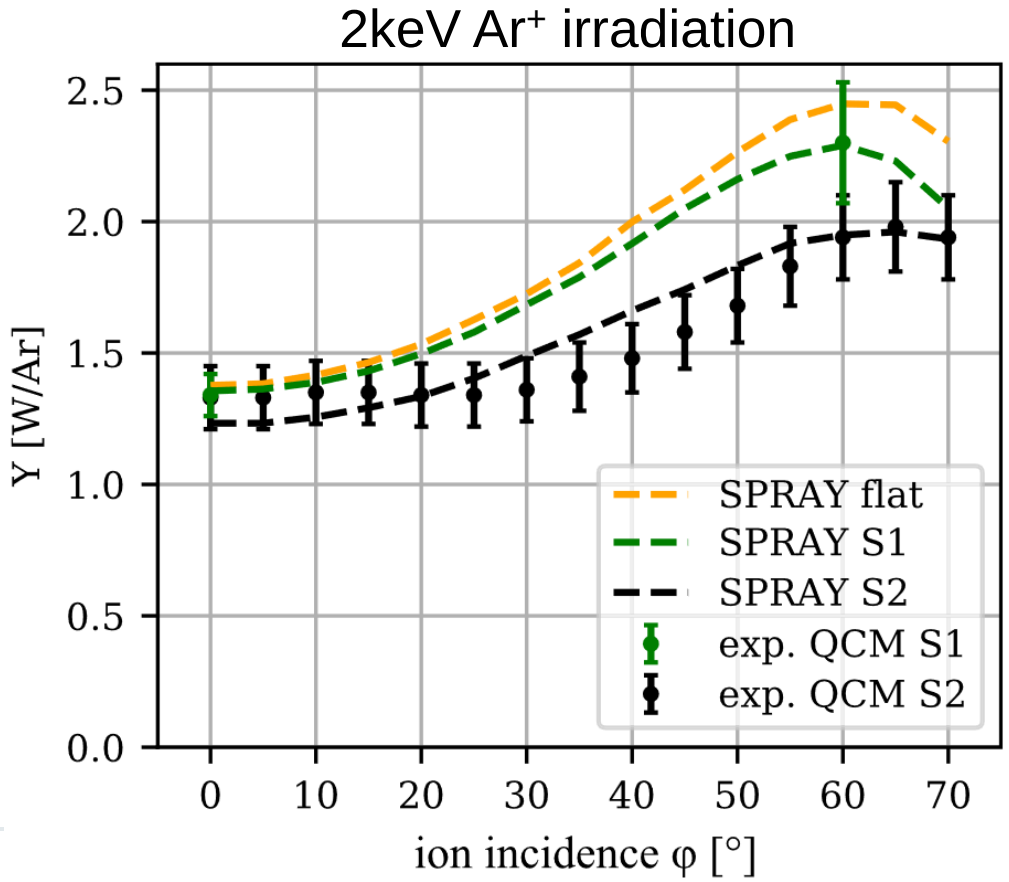
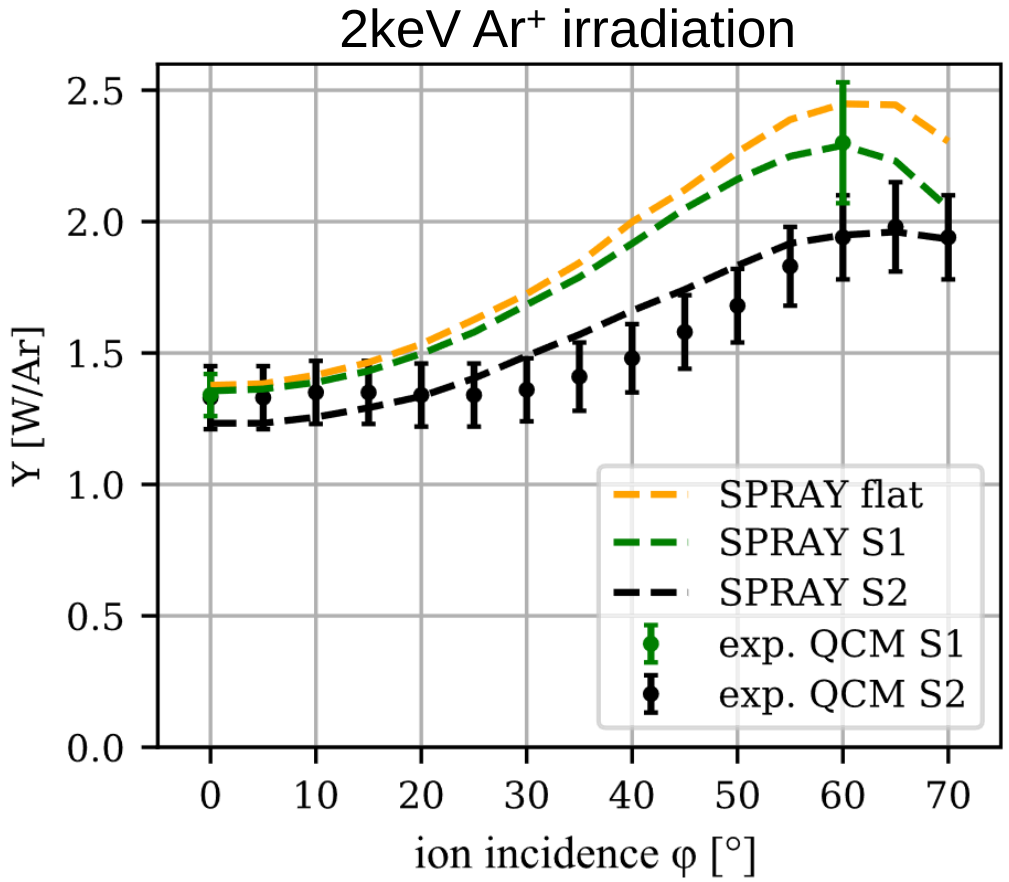


C. Cupak et al., Appl. Surf. Sci. 570 (2021)

Selected Results and Outlook

Gaussian rough surfaces:

- absolute values of sputter **yields are reduced** due to roughness effects
- angular dependence is smeared out
- results were used to **benchmark SPRAY** code

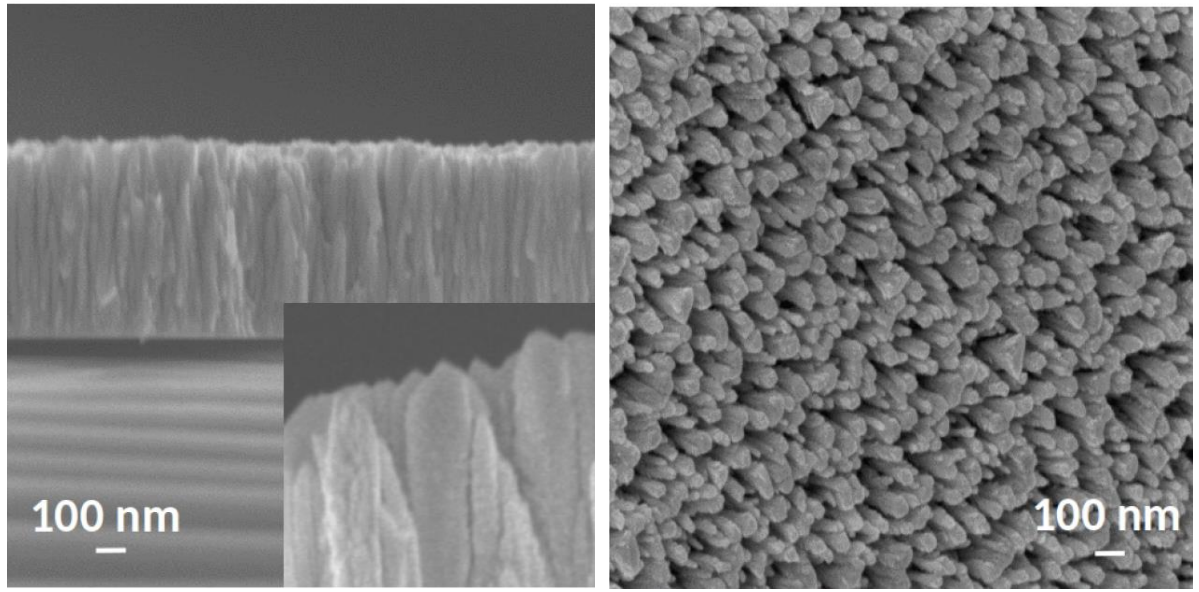


C. Cupak et al., Appl. Surf. Sci. 570 (2021)

Selected Results and Outlook

Nano-columnar surfaces:

sample creation:



Raquel González-Arrabal

A. Lopez-Cazalilla & C. Cupak et al., Phys. Rev. Mater. 6 (2022)

Selected Results and Outlook

Nano-columnar surfaces:

Molecular dynamics simulations:

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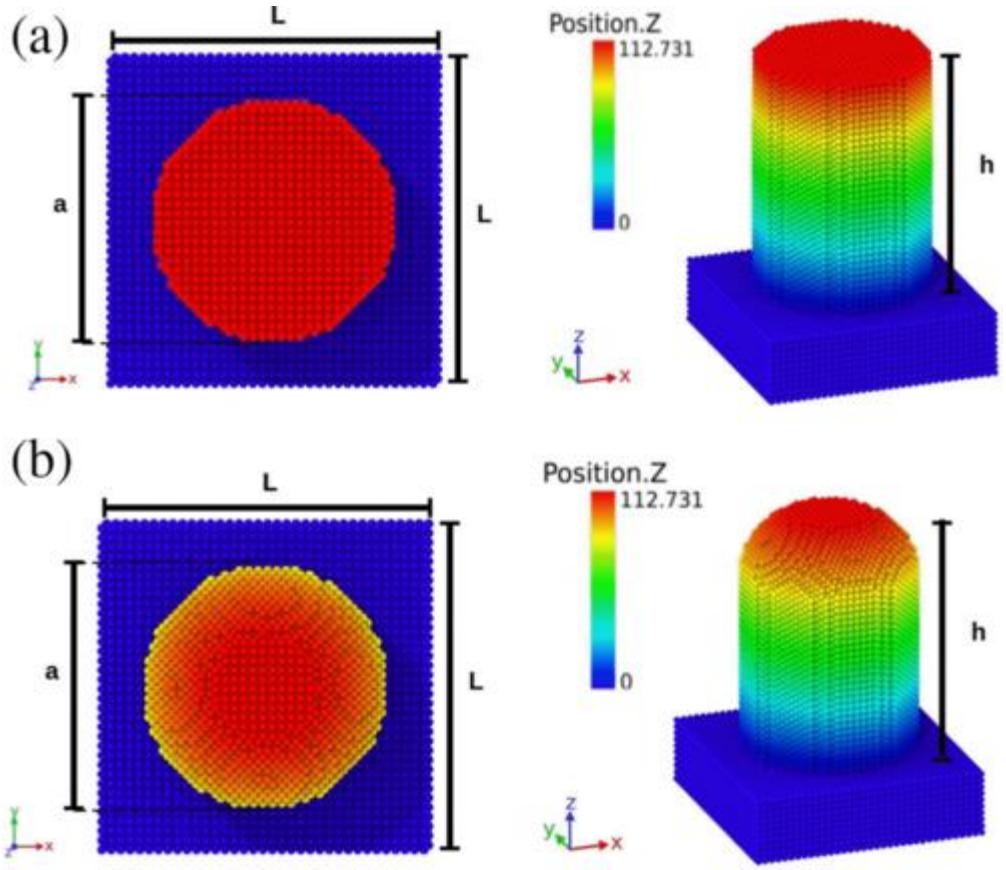


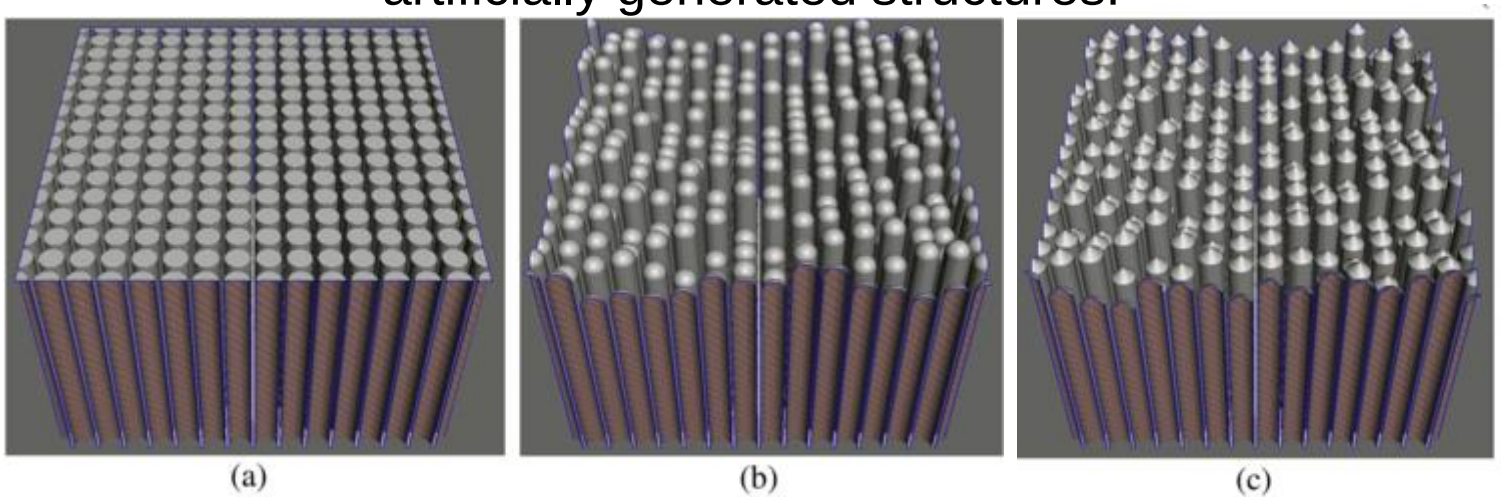
A. Lopez-Cazalilla & C. Cupak et al., Phys. Rev. Mater. 6 (2022)

Selected Results and Outlook

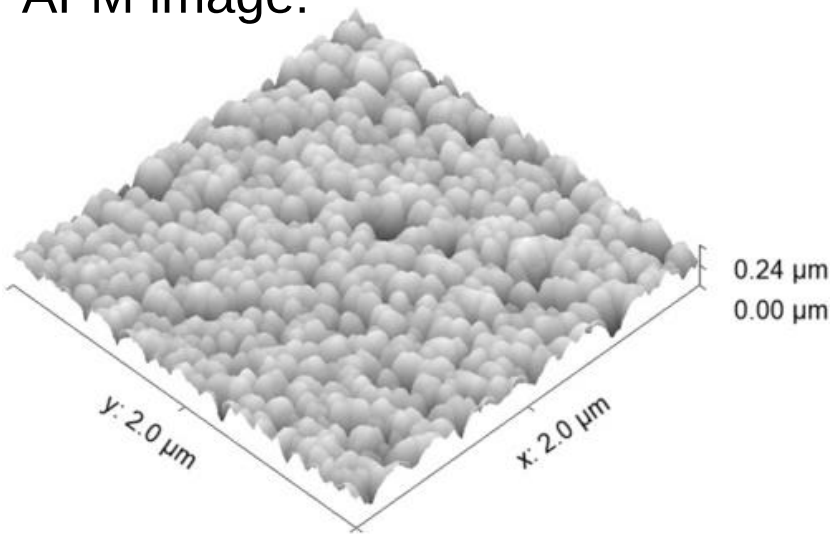
Nano-columnar surfaces:

SPRAY simulations:

artificially generated structures:



AFM image:

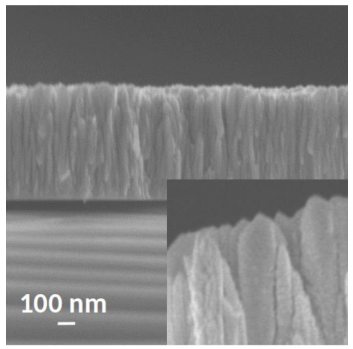


A. Lopez-Cazalilla & C. Cupak et al., Phys. Rev. Mater. 6 (2022)

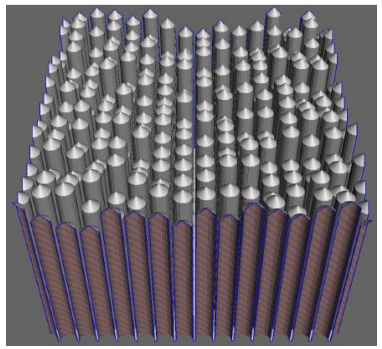
Selected Results and Outlook

Nano-columnar surfaces:

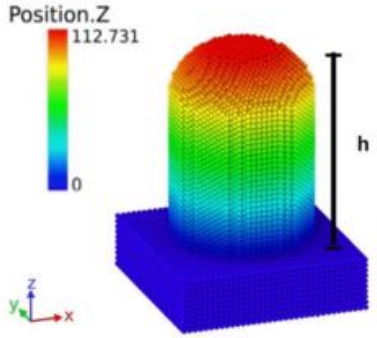
SEM image

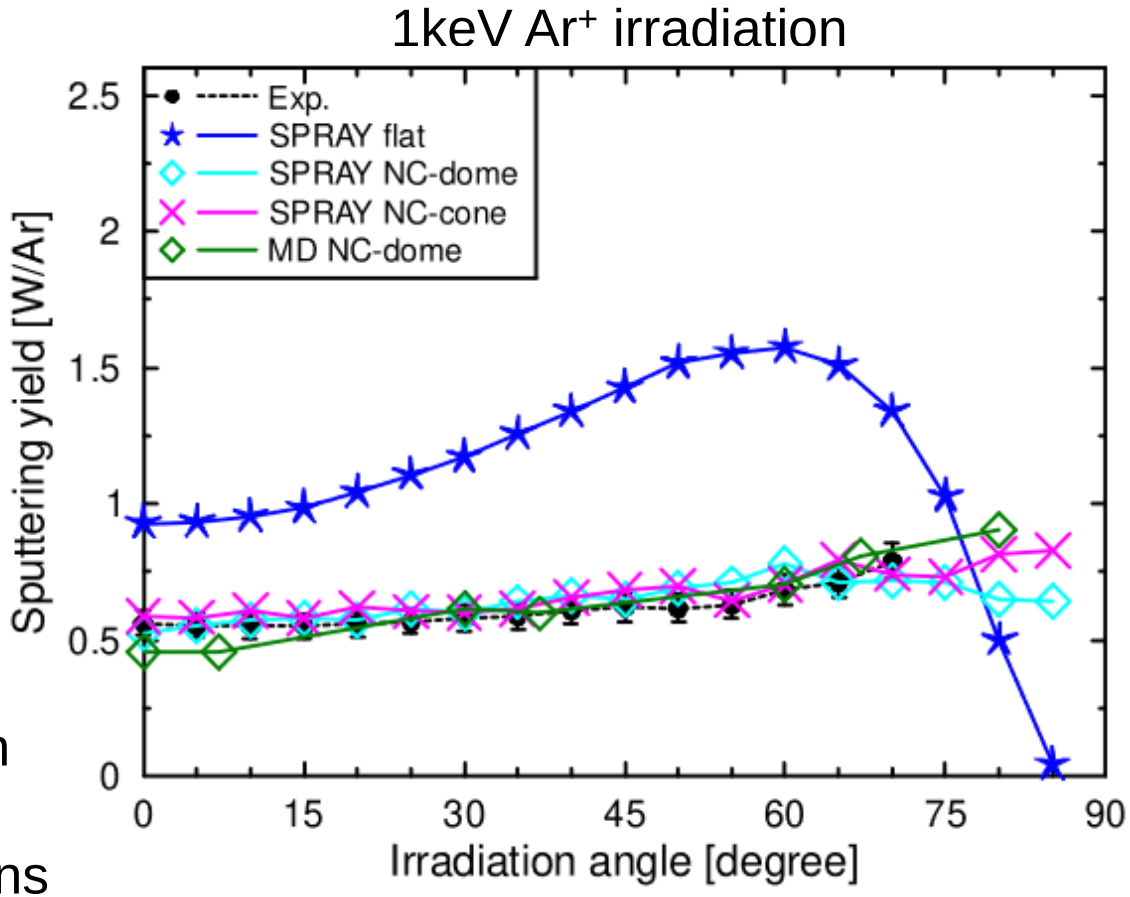


SPRAY input



MD input





→ very good agreement between **experimental** data, **SPRAY** simulations and **MD** Simulations

A. Lopez-Cazalilla & C. Cupak et al., Phys. Rev. Mater. 6 (2022)

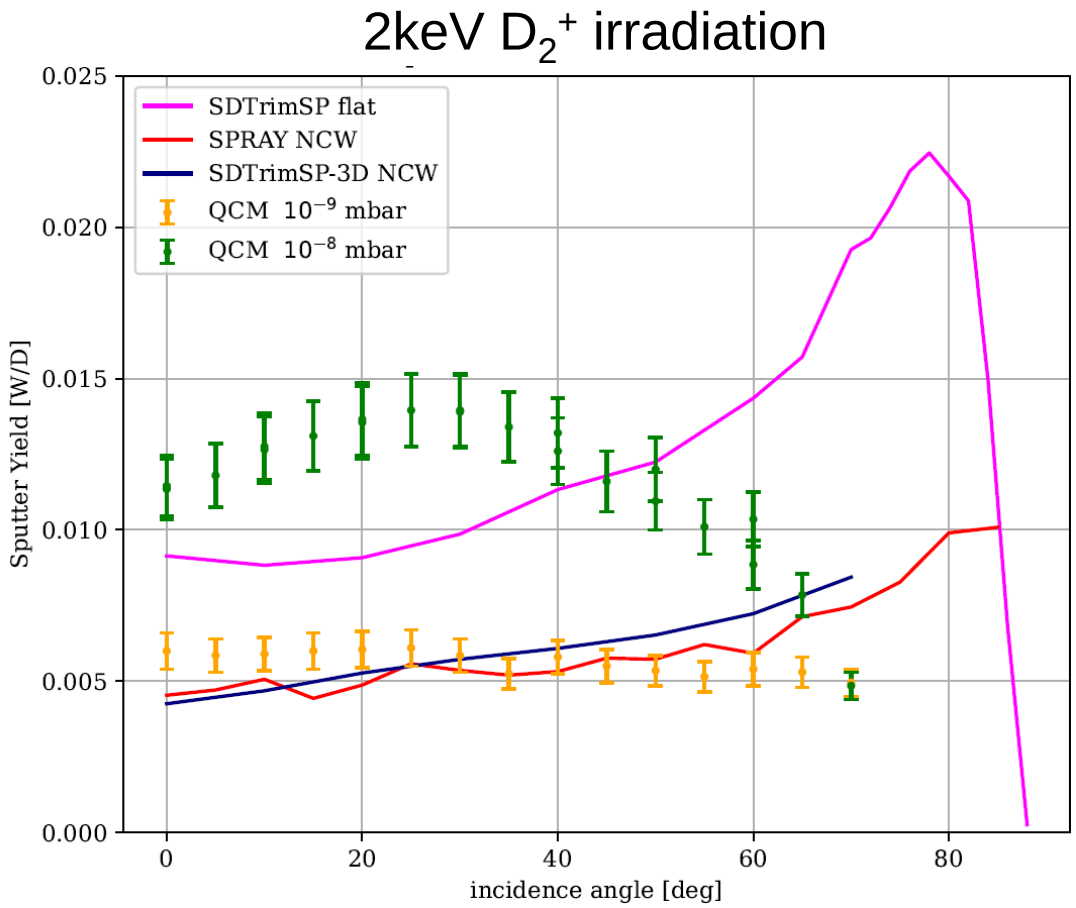
Selected Results and Outlook

Nano-columnar surfaces:

→ pronounced effect due to residual gas pressure in experimental data

→ mass reduction signal represents a convolution of **W sputtering and absorbate sputtering**

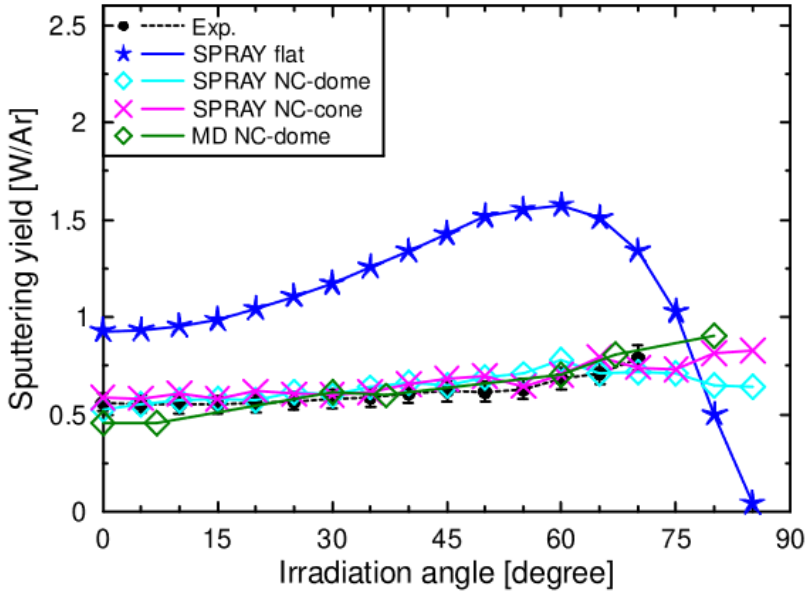
→ sputter yield reduction due to **geometry effects only** (no particle transmission)



Selected Results and Outlook

Nano-columnar surfaces:

→ can we **optimize** this structure further?

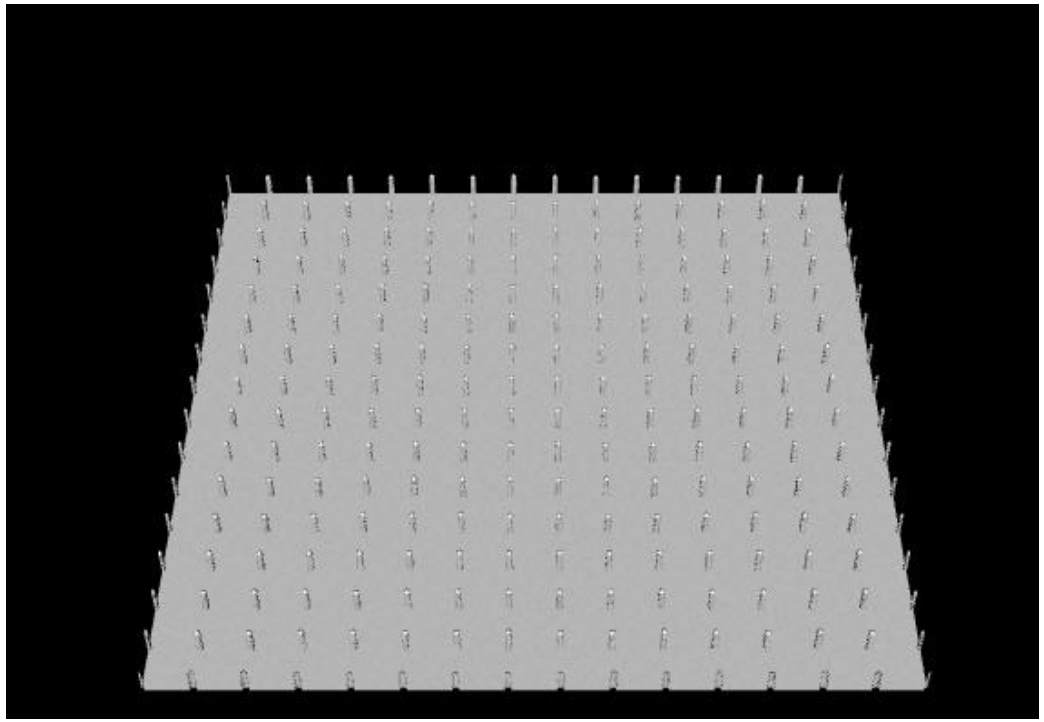


Selected Results and Outlook

Nano-columnar surfaces:

→ can we **optimize** this structure further?

- **vary shape parameters** (height, areal density, …) to minimise sputter yields
- investigate optimized structure in QCM experiments



Selected Results and Outlook

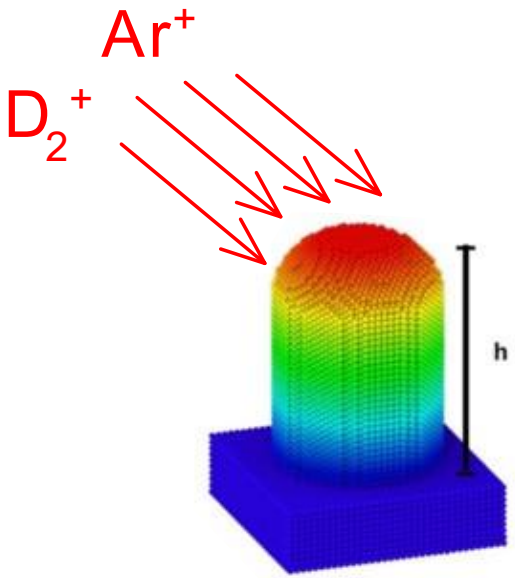
Nano-columnar surfaces:

→ can we **optimize** this structure further?

- **vary shape parameters** (height, areal density, …) to minimise sputter yields
- investigate optimized structure in QCM experiments

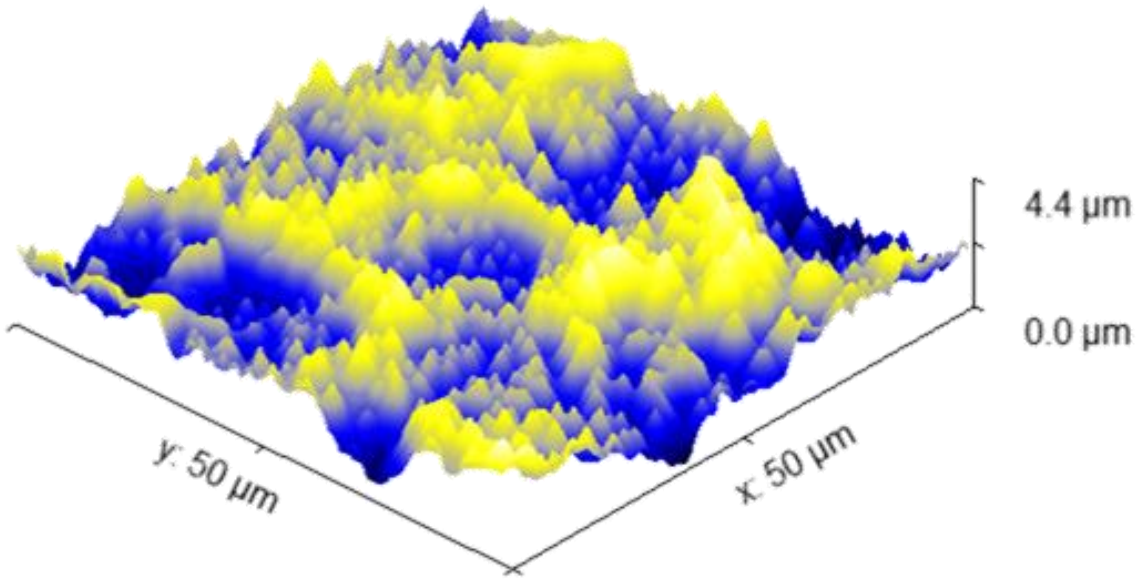
→ how **stable** can such a structure be?

- investigate **long term erosion** properties of nano-columns in experiment and simulation



Selected Results and Outlook

Pyramidal surfaces:



→ **pyramidal W surfaces** grown on Si substrates in Milan

→ surfaces can be investigated with **catcher setup**

→ support experimental data with **numerical simulations**

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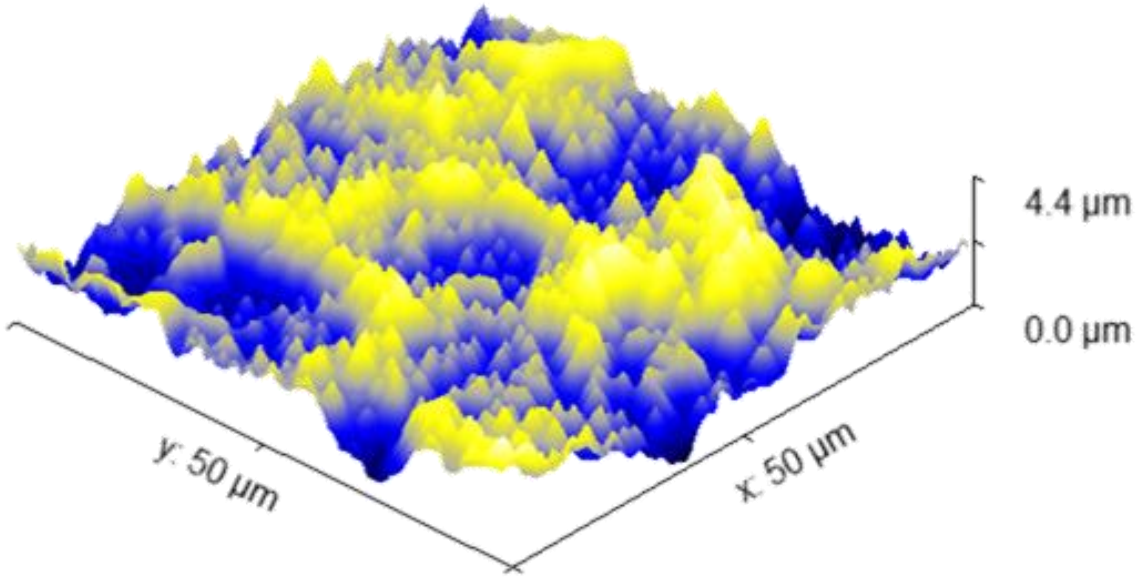

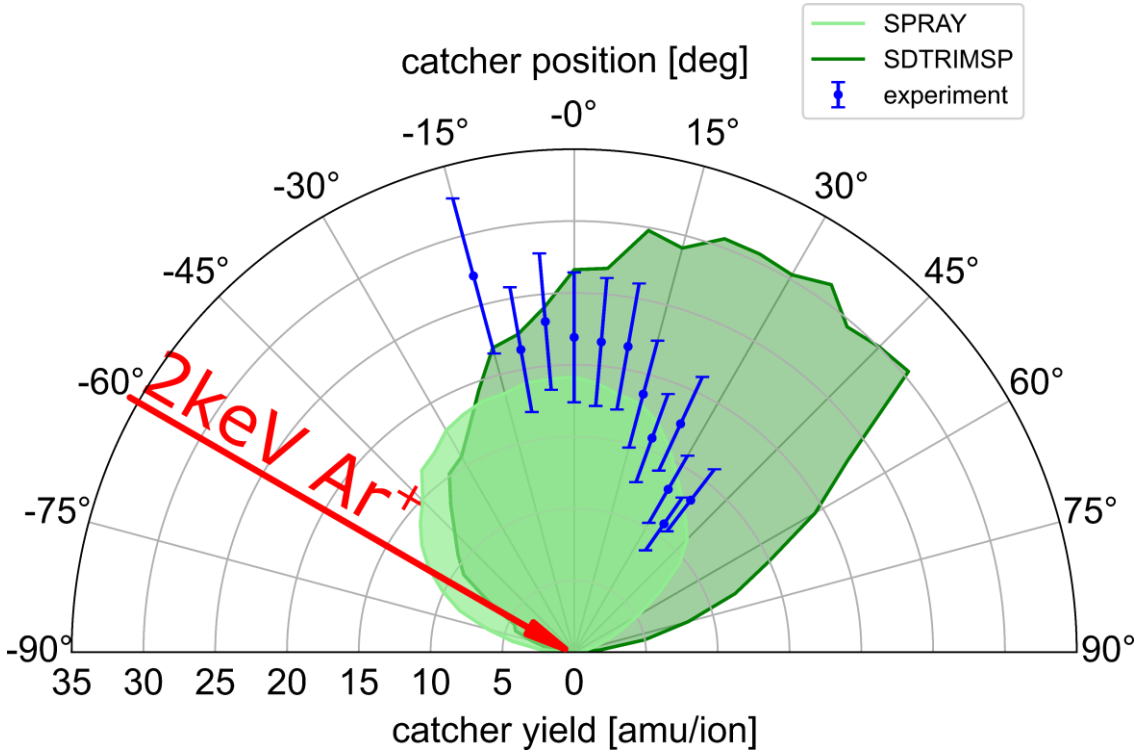

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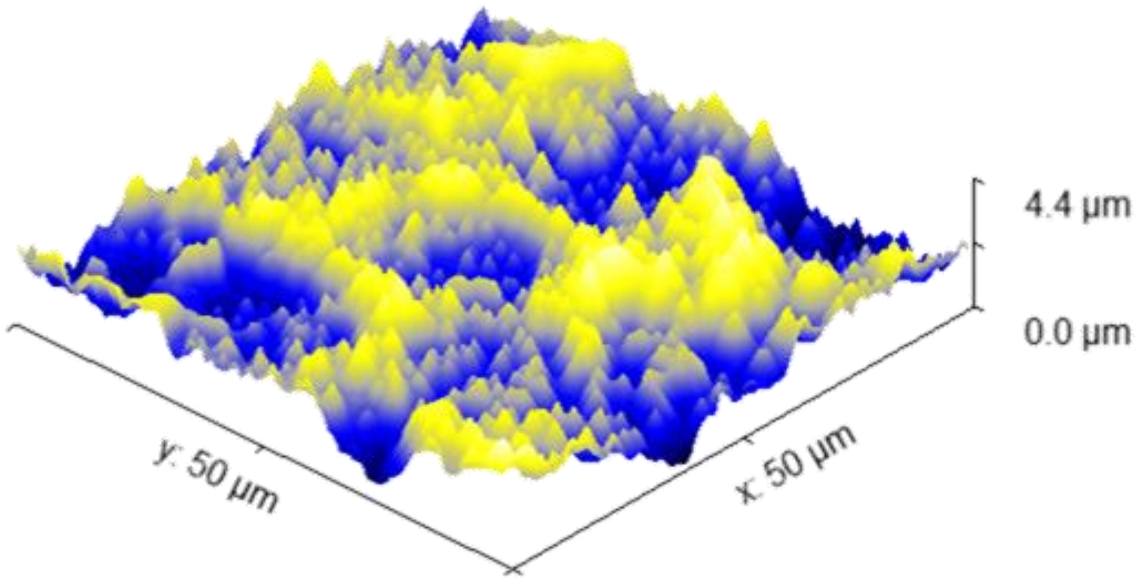

→ investigate **different** pyramidal **heights**

→ compare to catcher data for flat surfaces

→ investigate how **sputtering into the direction of the ion beam** is triggered

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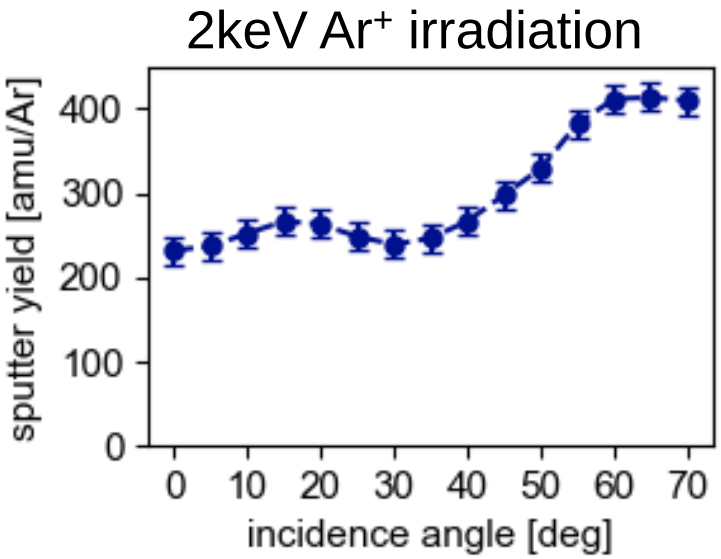
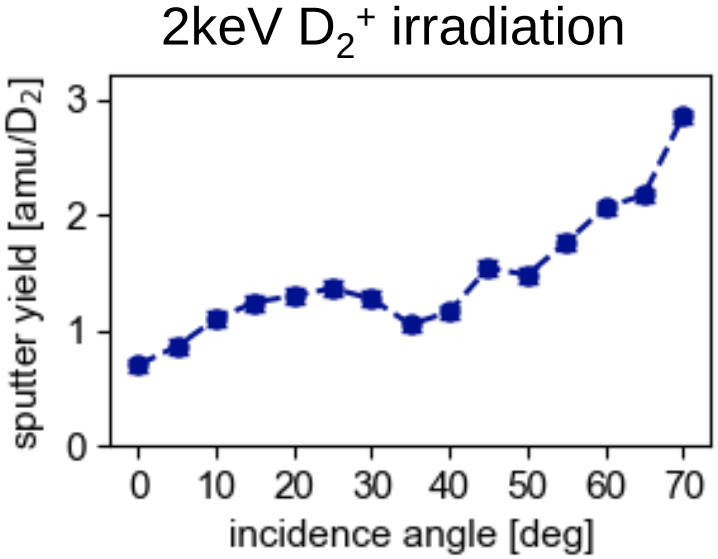
Selected Results and Outlook

Re-deposited surfaces:

original W sample:

→ sample creation:
PVD - grown at
IPP Garching





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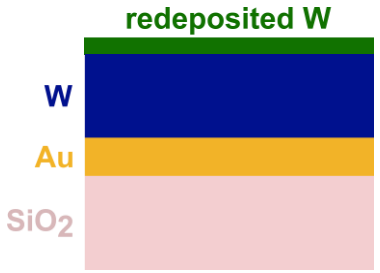
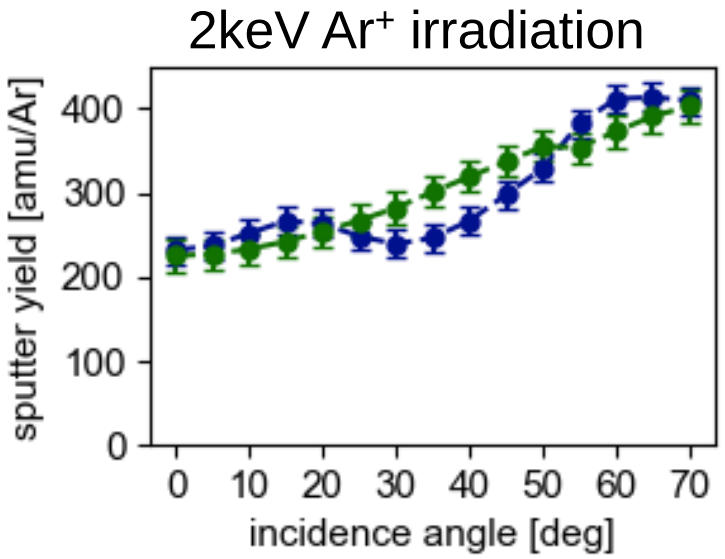
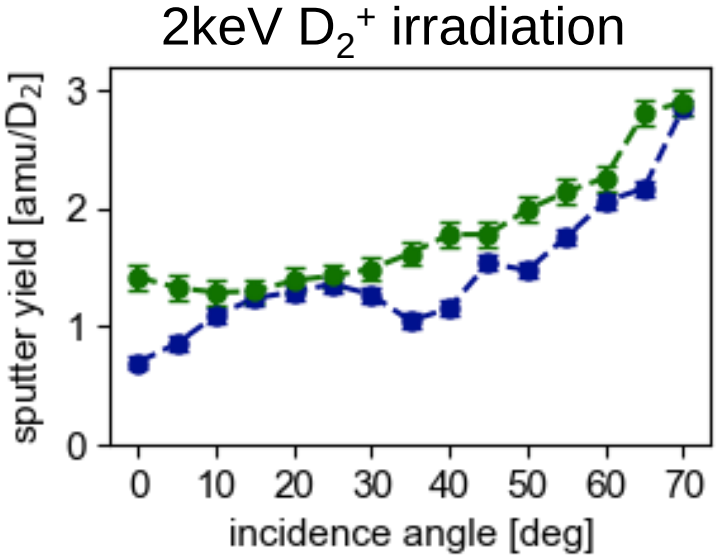
original W sample:

redeposited W sample:







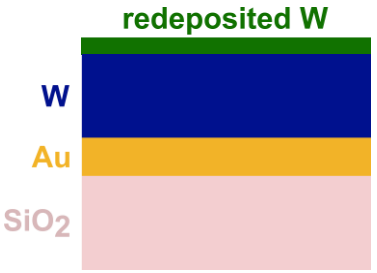
→ sample creation: sputter coating at TU WIEN

Selected Results and Outlook

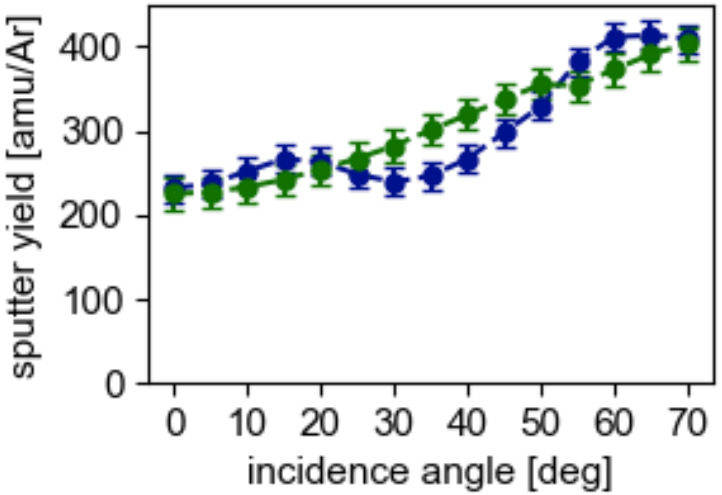
Re-deposited surfaces:

original W sample:

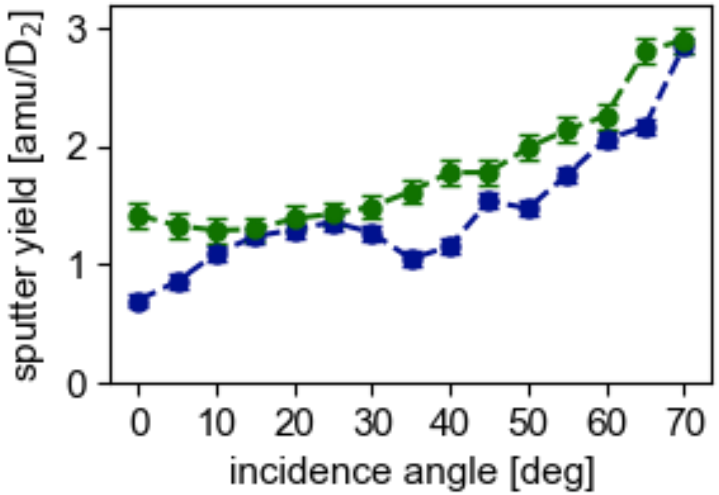
re-deposited W sample:



2keV Ar^+ irradiation



2keV D_2^+ irradiation



→ absolute sputter yield values of re-deposited and original layers are comparable

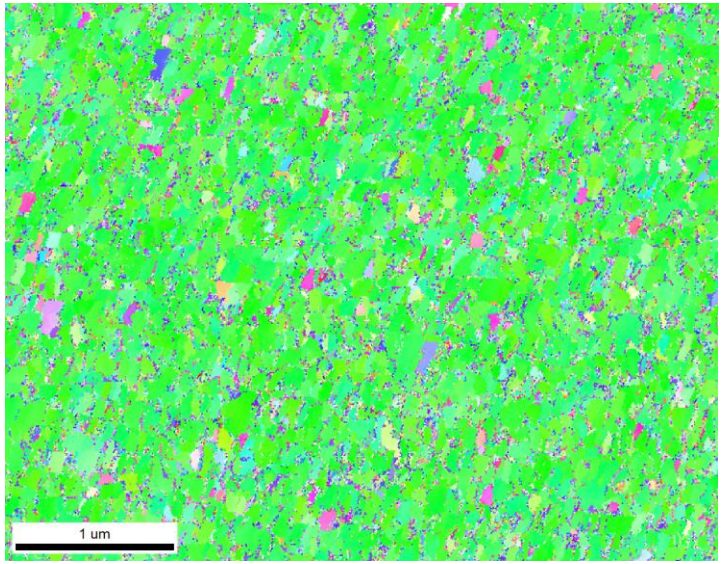
→ **local minimum** found in original W layers

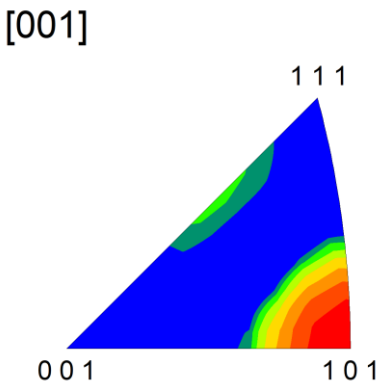
→ minimum not visible any more for re-deposited layers

TEXTURE EFFECTS?

TEXTURE EFFECTS?

EBSD map of representative Fe QCM sample:





→ ions can penetrate deeper into the material for specific incidence angles

→ collision cascade is triggered at higher depths

→ amount of **effectively sputtered particles** can be **reduced**

Selected Results and Outlook

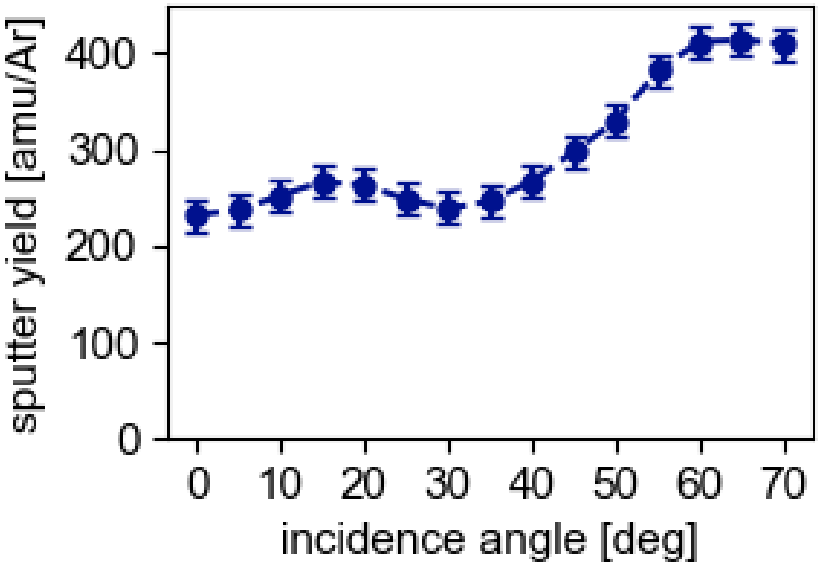
Surfaces with specific textures:

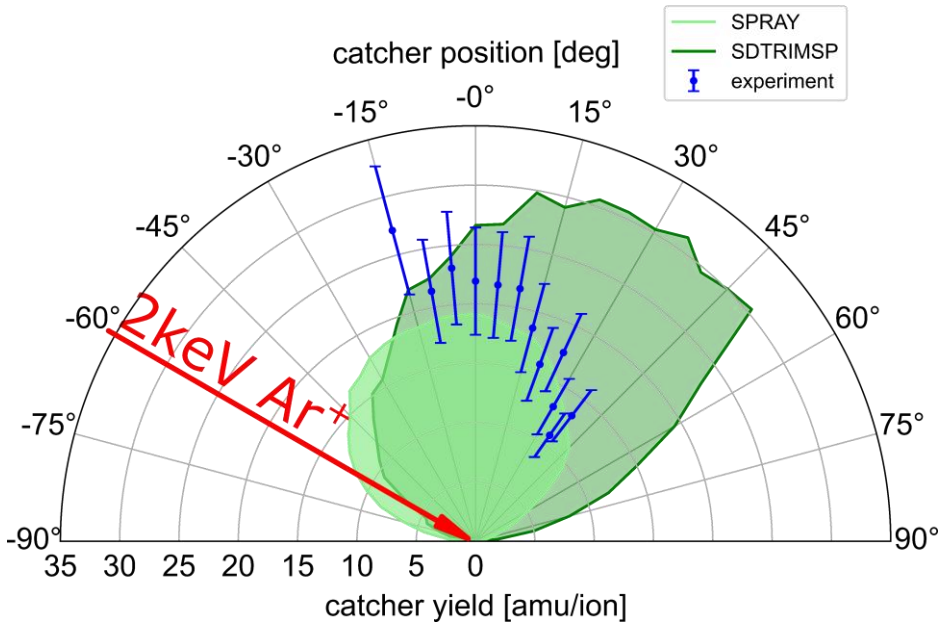
→ **crystallographic features** seen in previous samples

→ check on minima and maxima in angular dependent sputter yields and if they correlate with **specific** crystallographic **orientations**

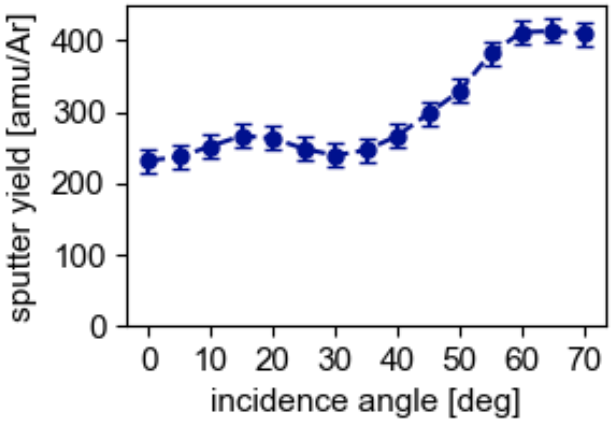
→ investigate different **materials**, different **projectiles** with variable **energies**

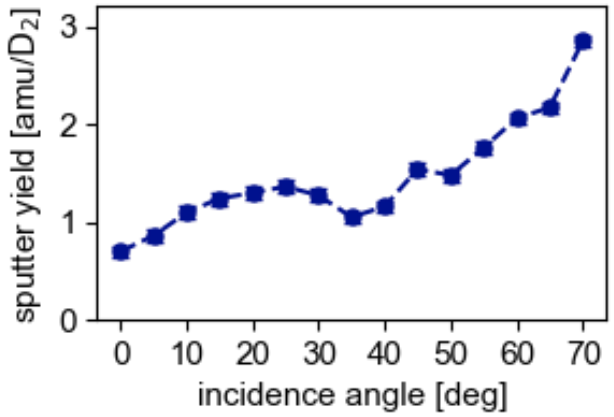
→ investigate also **emission characteristics** of sputtered particles for various textures





TEXTURE EFFECTS?





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