Max-Planck-Institut für Plasmaphysik

SDTrimSP-3D based erosion modelling considering roughness

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EUROfusion

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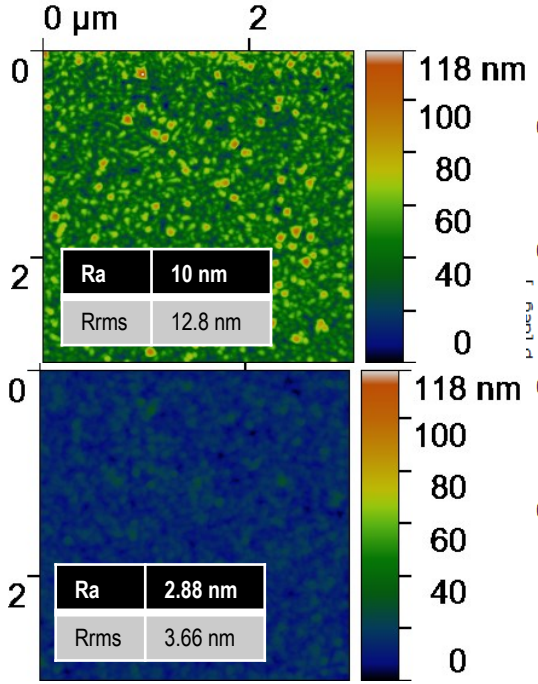
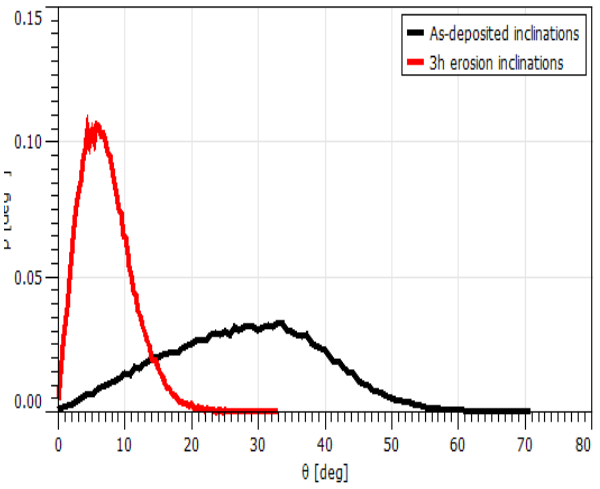
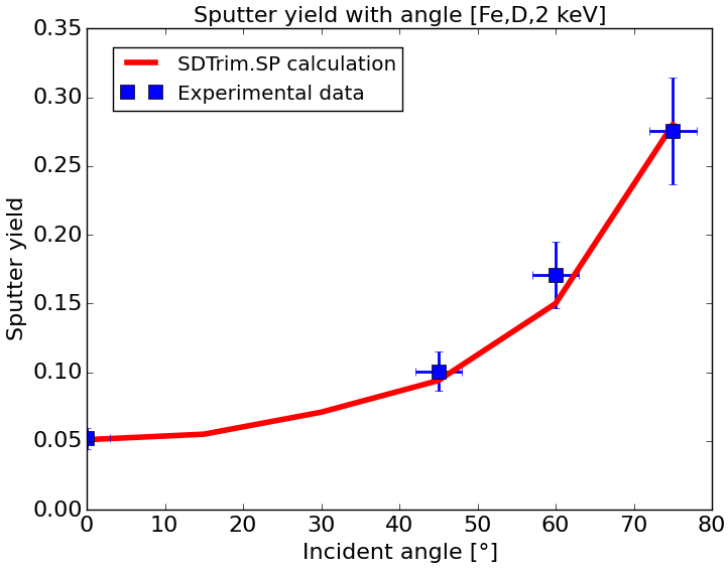
Motivation

- **Sputter yield & reflection data from surface-physics experiments**
  - Large data-base of sputter-yields (Y), reflection yields (R) and energy reflection coefficients R_E
  - Drawback:
    - Almost all are from well-prepared samples → do not match PFC-properties
    - (Few) Experiments with technical grade samples yield averaged values (Y only)
- **Now: capability to derive Y, R, R_E from static & dynamic simulations (2D & 3D)**



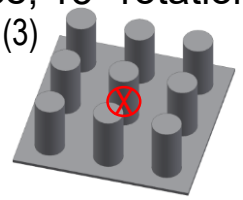




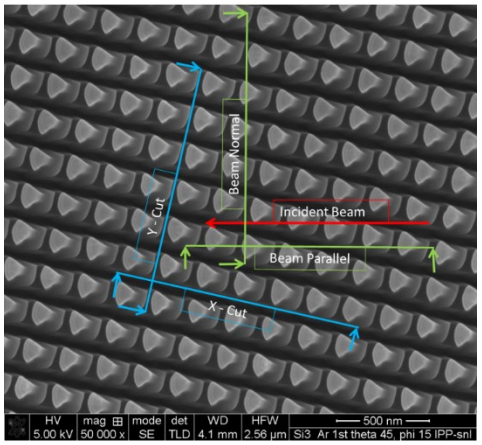
Si – 45° incidence, 15° rotation

SDTrimSP-3D Si columns eroded by 5 keV Ar under 45° incidence, 15° rotation

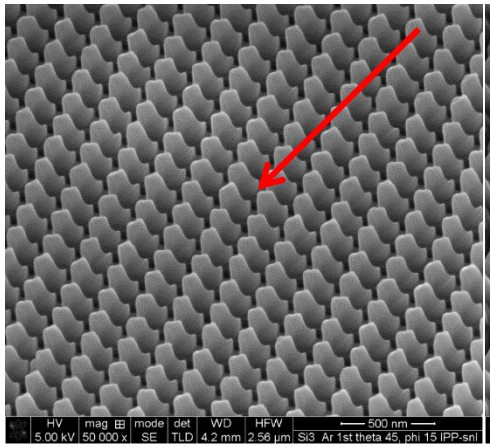
(3)



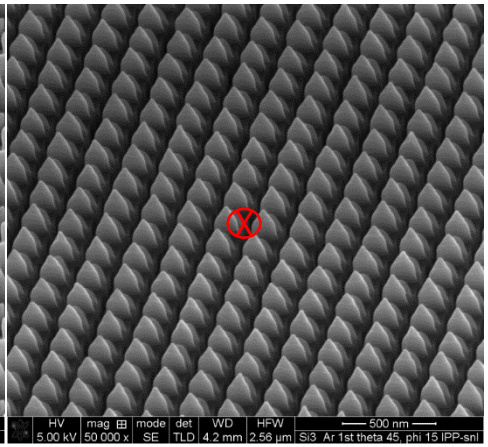
Birds-eye view



Tilted view



Tilted, rotated 90°

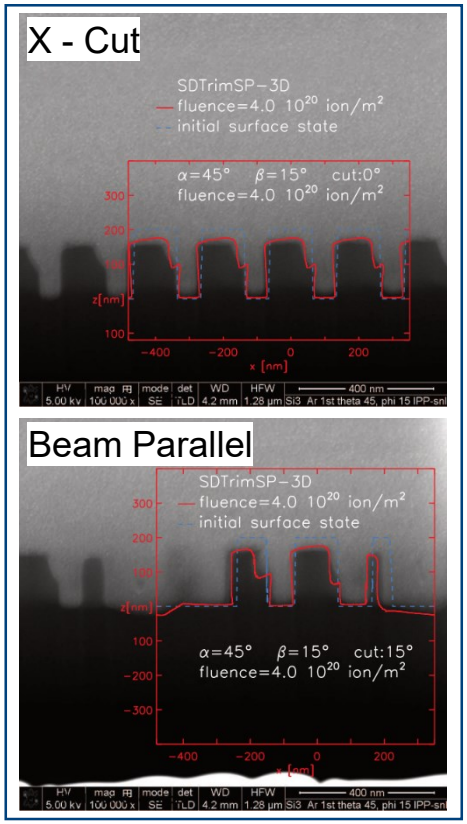


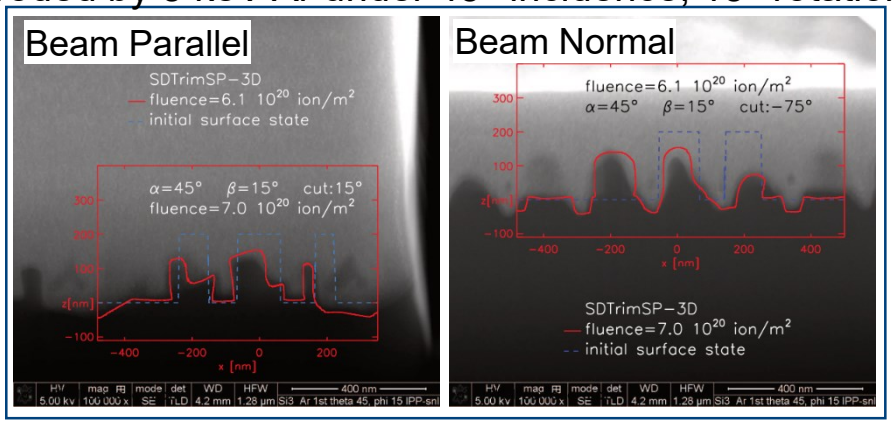
X = 5 (max)

6.1×10^{20} Ar/m²

Si – 45° incidence, 15° rotation

SDTrimSP-3D Si columns eroded by 5 keV Ar under 45° incidence, 15° rotation



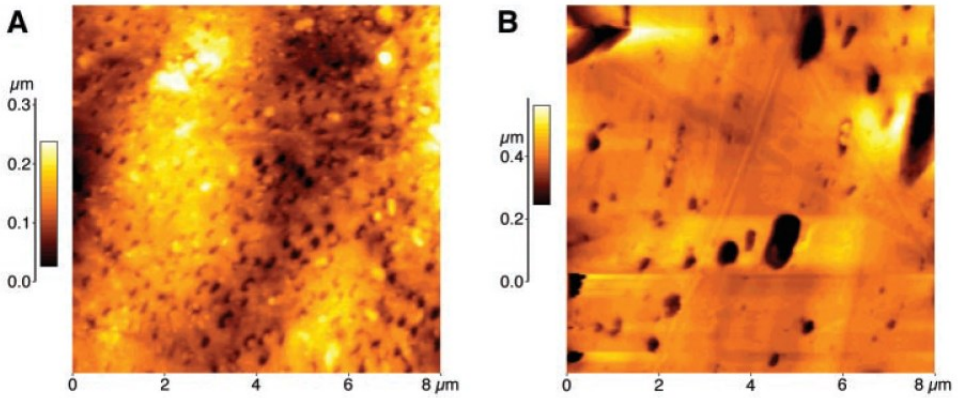


Overall good qualitative agreement

Project

- **Key issues**
  - Simulations are expensive (especially 3D) & yield huge amount of data
  - Parameter explosion (surface topology) vs E, impact angle in 1D
  - Standard surface description like RMS is utterly incomplete: same RMS from very different structures:

(e.g. Sciene 297 (2002), p. 973-976)



- **→ Different description is mandatory (but needs to be useful for relevant surfaces)**
  - Characterisation of surface structures via
    - Frequency spectrum (Fourier transform) or
    - Autocorrelation function (ACF)

$$\mathrm{ACF}(x,y) = \frac{\int\int \rho(x-x', y-y') \times \rho(x', y')dx'dy'}{\int\int \rho^2(x, y)dxdy}$$

  - Both measures suited also for technical surfaces (ripples, grinding patterns)

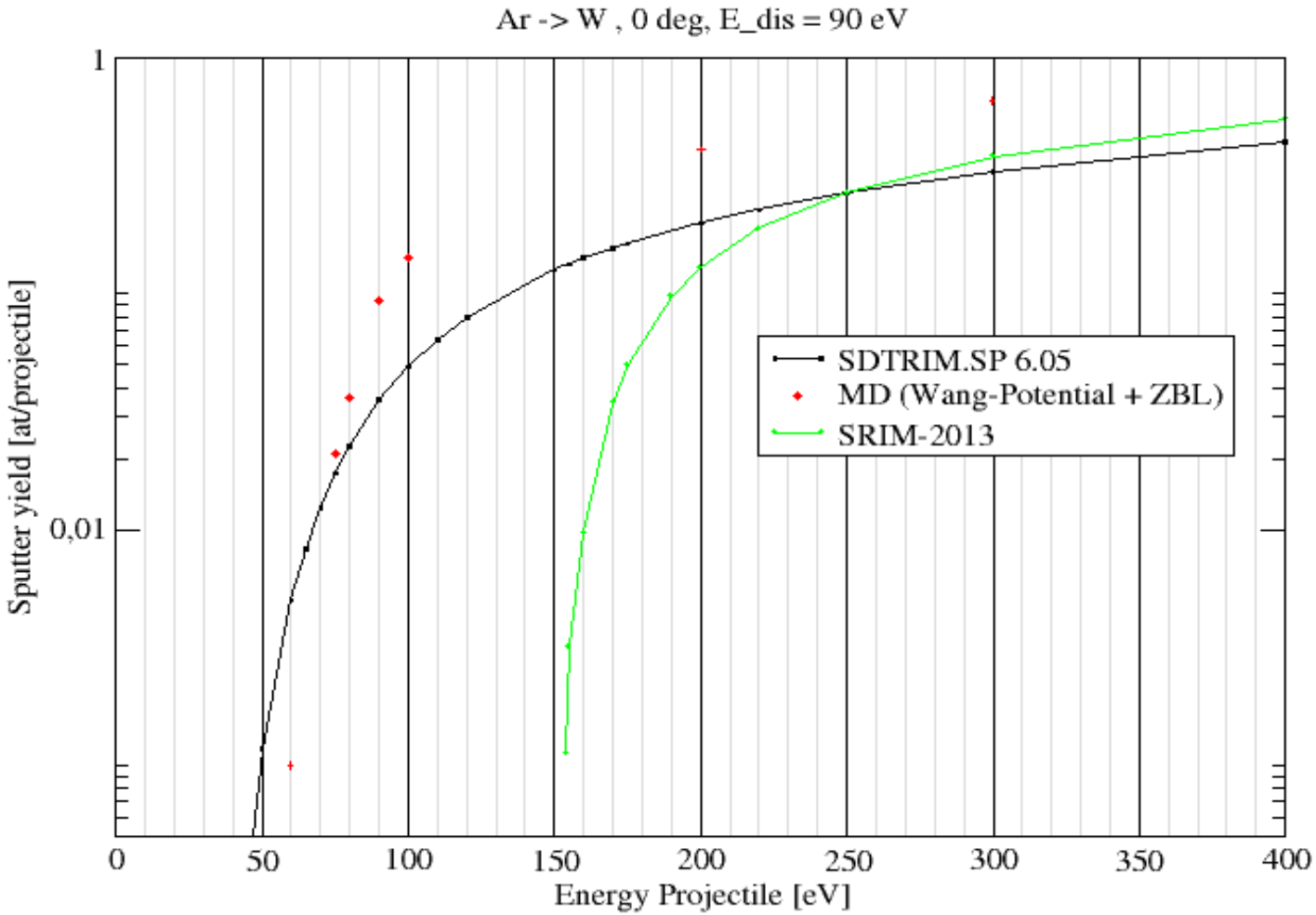
Project

- **Simulations (task)**
  - Synthesize surfaces with known FFT and ACF
  - Simulate static and dynamic sample-ion-interaction
  - Extract Y, R, R_E and (try to) correlate with surface properties
  - Investigate fluence (=time) dependent evolution equations in FFT/ACF-space

- **Verification experiments**

  (timeline/exp. depending on availability of masterand – exp. facilities are present)
  - Exposure of microstructured samples
    - Surfaces precharacterized with
      - AFM
      - SEM
      - Confocal microscopy
    - Exposure to ion beam (fixed energy and projectile), parameters:
      - Impact angle
      - Fluence

Project


Ar -> W , 0 deg, E_dis = 90 eV
Sputter yield [at/projectile]
1
0,01
0
50
100
150
200
250
300
350
400
Energy Projectile [eV]
SDTRIM.SP 6.05
MD (Wang-Potential + ZBL)
SRIM-2013