Surface morphology and structure: Experiments, SDTrim-simulations and Surrogate modelling

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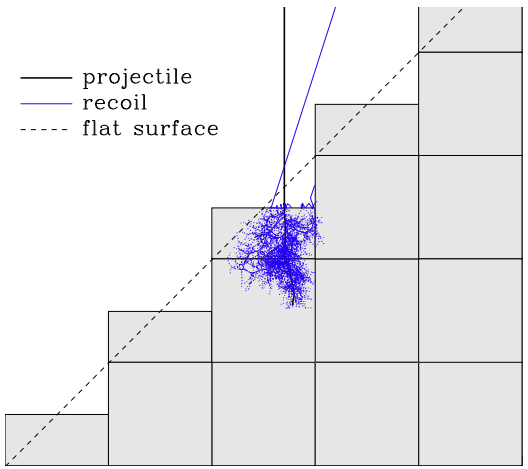
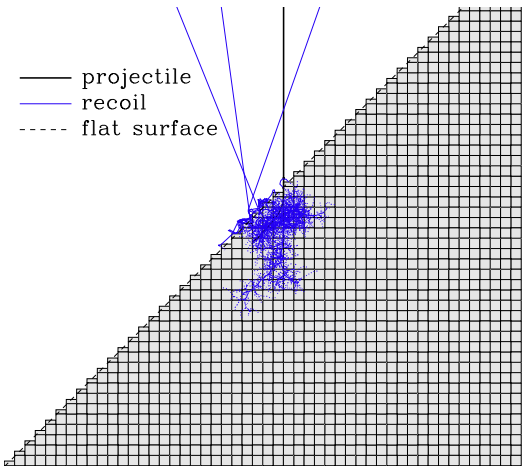
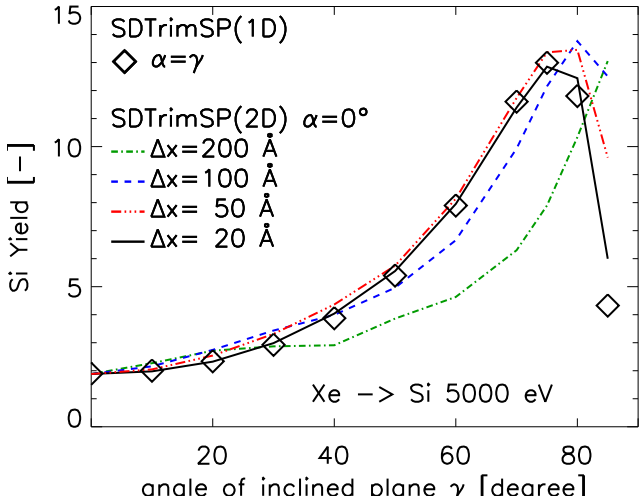
06 May 2022

Fundamentals

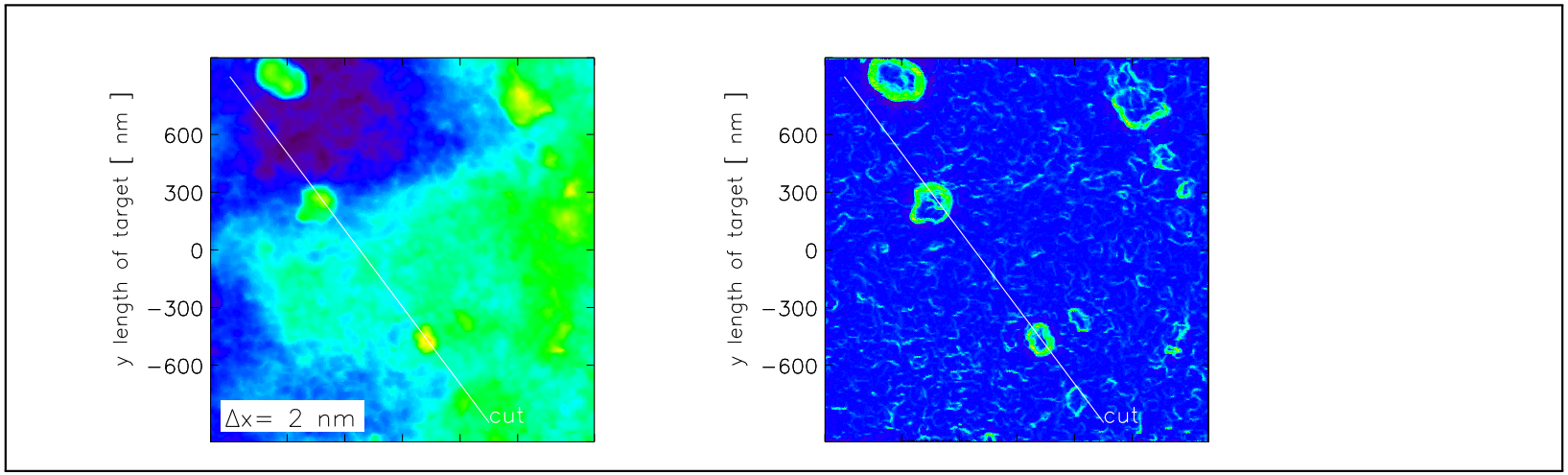


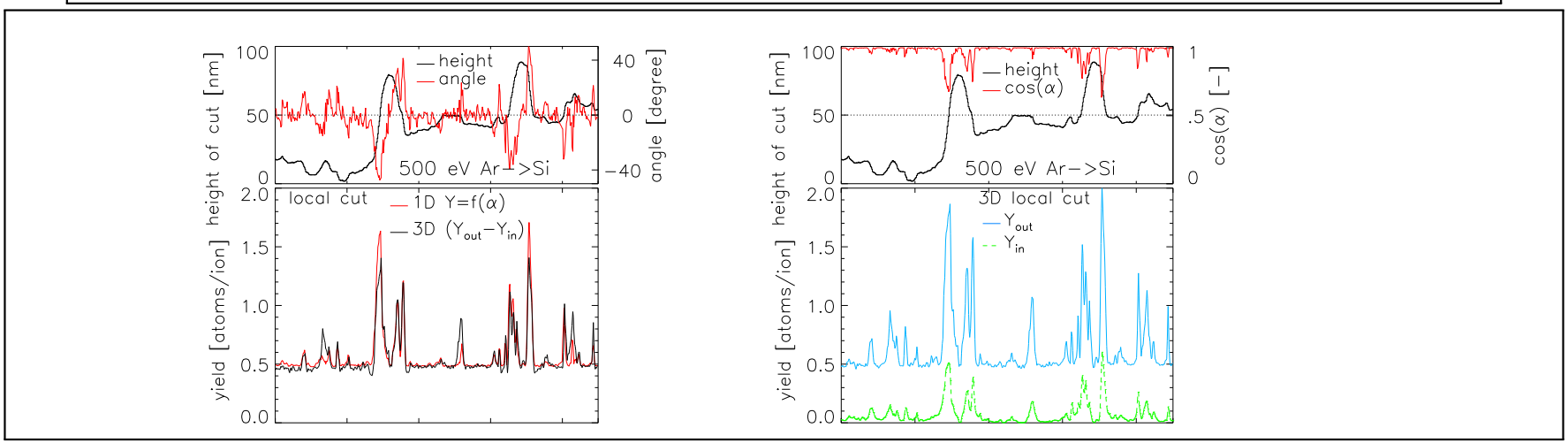




- Local sputter yield Y(x) depends on local impact angle $\alpha(x)$
- 'Local' : O(size of collision cascade)
- BCA-Codes like SDTrimSP-2D, SDTrimSP-3D, TRI3DYN or MD are suited tools

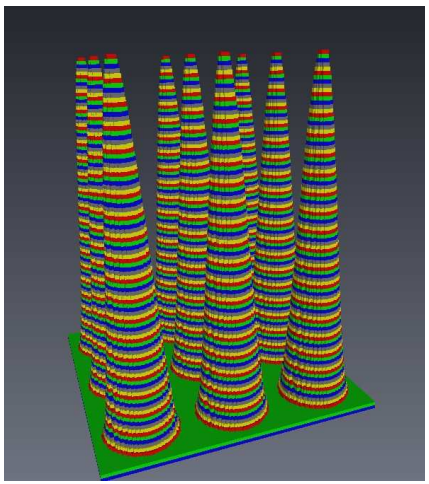
Fundamentals

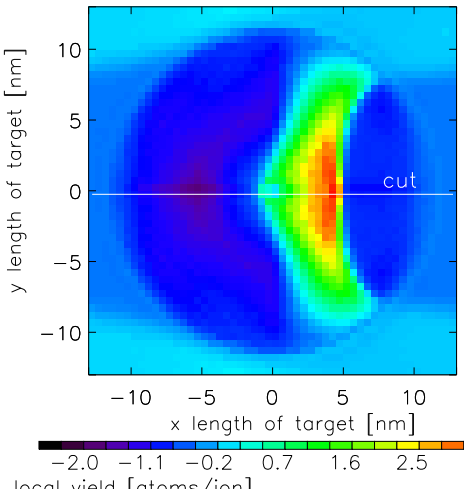


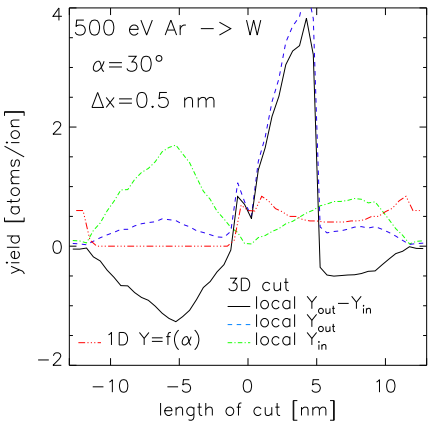


- Simplest approximation : $Y_{total} = \int dxdy Y\left(\alpha\left(x,y\right)\right)$
- Used since decades : Küstner (1998), . . . , Szabo (2022)
- Limits are known : contribution of redposition, shadowing

Fundamentals



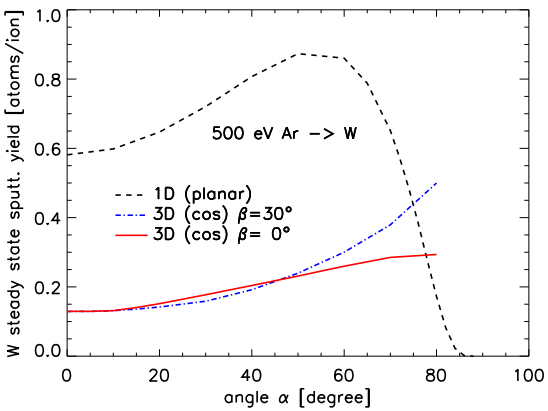




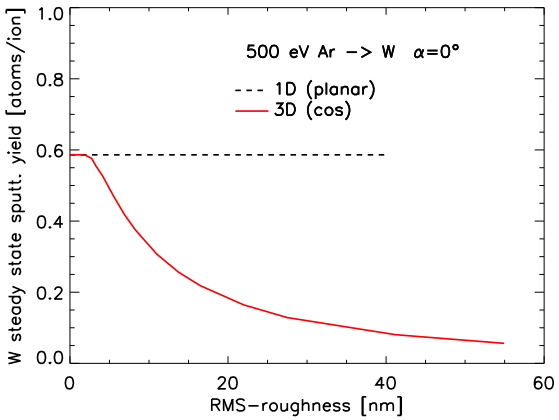
- SDTrim-3D simulations (c.f. Physica Scripta T170, 014056 (2017))
- SDTrim-3D later validated using predicitve simulations

Fundamentals

Sputtering of rough surfaces: A 3D simulation study 10



(a)

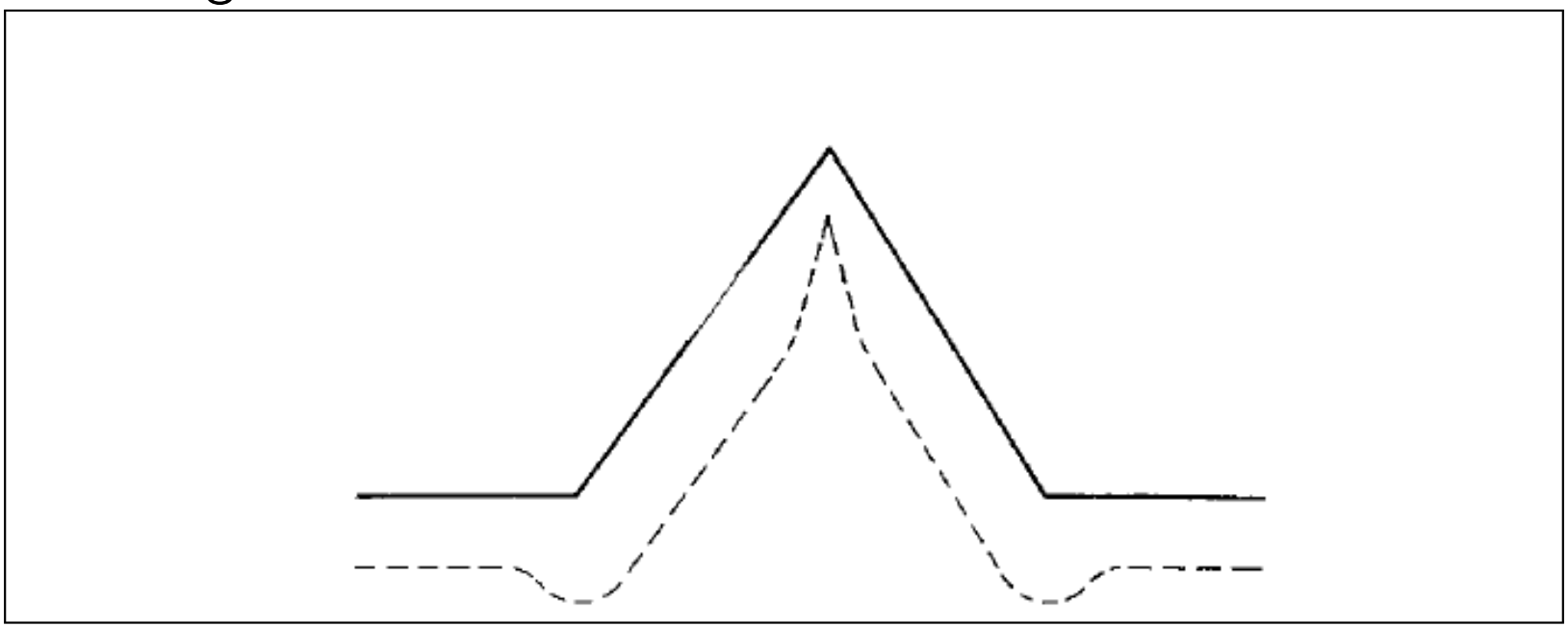


(b)

- General observation : slight roughness decreases net sputter yield

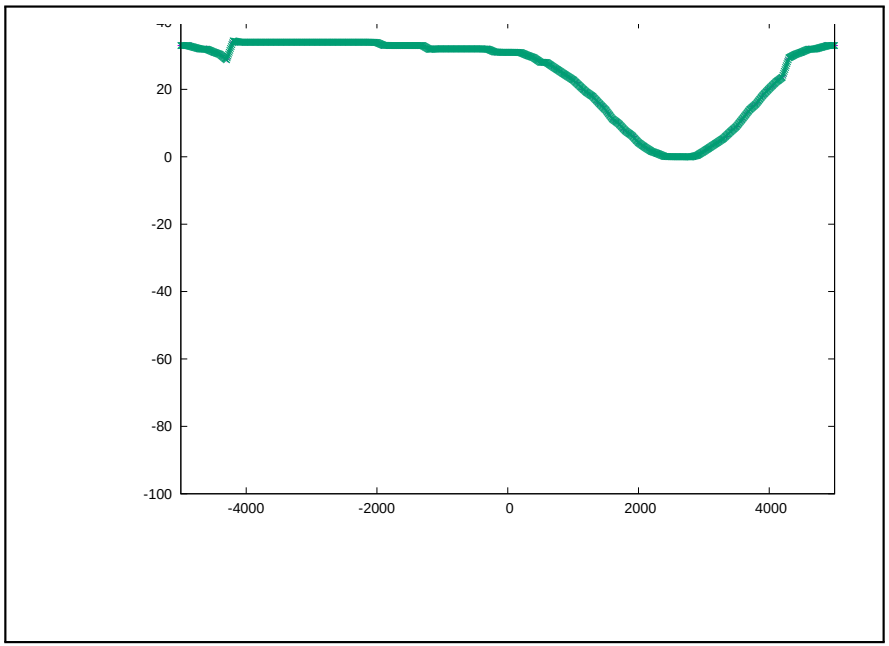
Surrogate Models

Impact angle good parameter for instantenious sputter yield estimates
Clearly insufficient for predictions (with fluence)
'Sigmund ridge' :



Surrogate Models

Impact angle good parameter for instantenious sputter yield estimates
Clearly insufficient for predictions (with fluence): Dynamics
Extend model to $Y(\vec{\alpha})$



5 keV Ar $\rightarrow$ Cu

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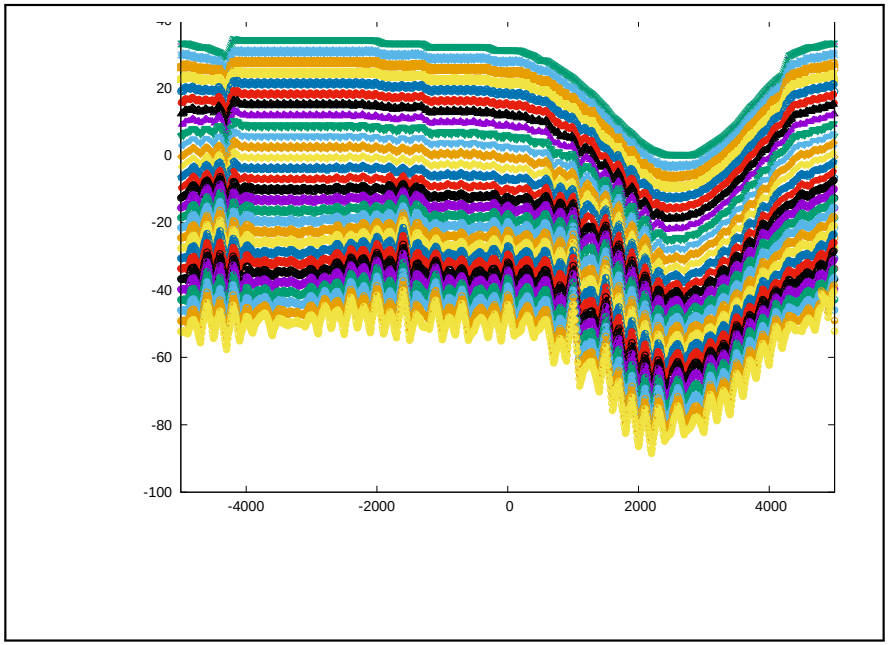

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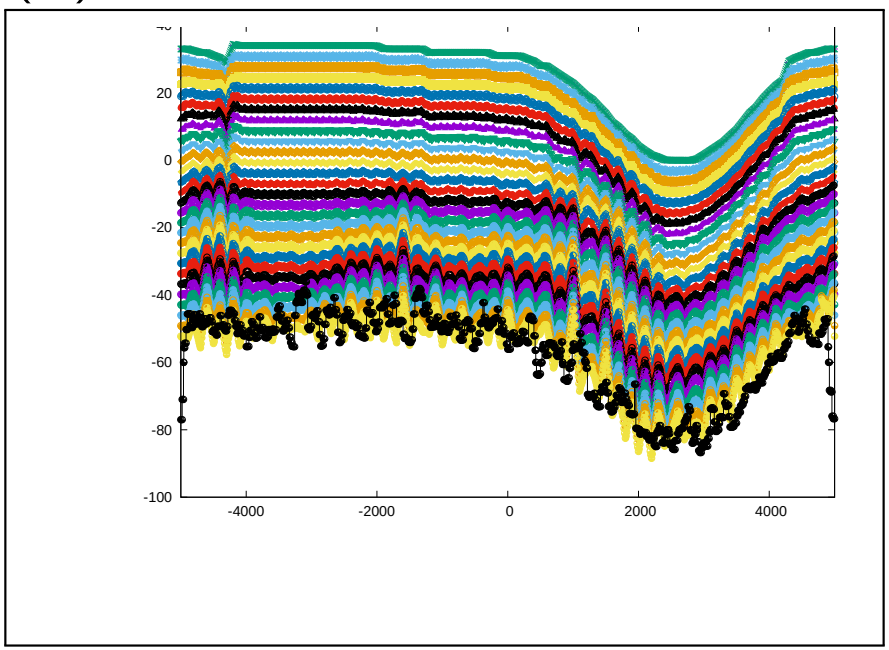


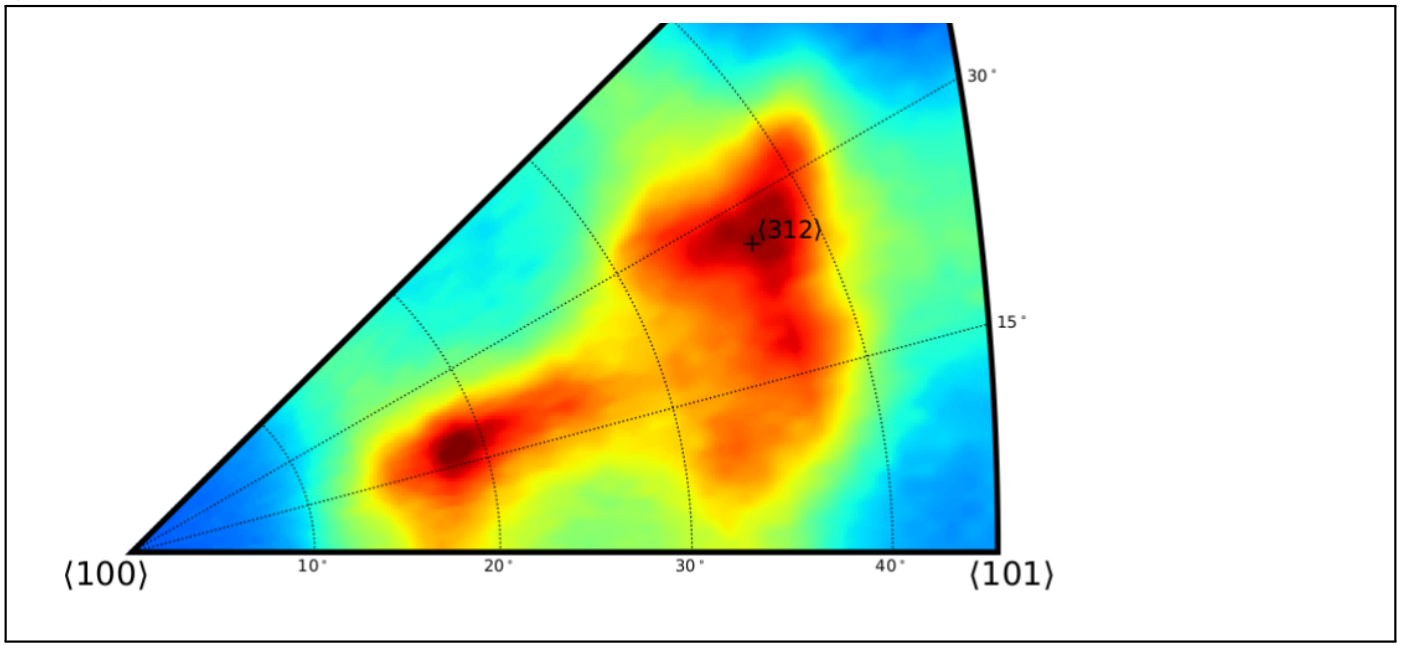
Fast linear (matrix) predictor in 1-D...extension two 2-D ongoing
But do not forget: heterogenous materials...

Experimental observations

Does the impact angle describe everything ?
Exposure of polished W/WfW to D and Ne $\rightarrow$ different morphologies and erosion depths
Angle distributions do not explain observed erosion depths!

Experimental observations

Does the impact angle describe everything ?
Sputtering yield depends on local atomic structure, i.e. amorphous or crystalline (see PhD Karsten Schlueter, subsequent PRL 2021):
30 keV Ga $\rightarrow$ W

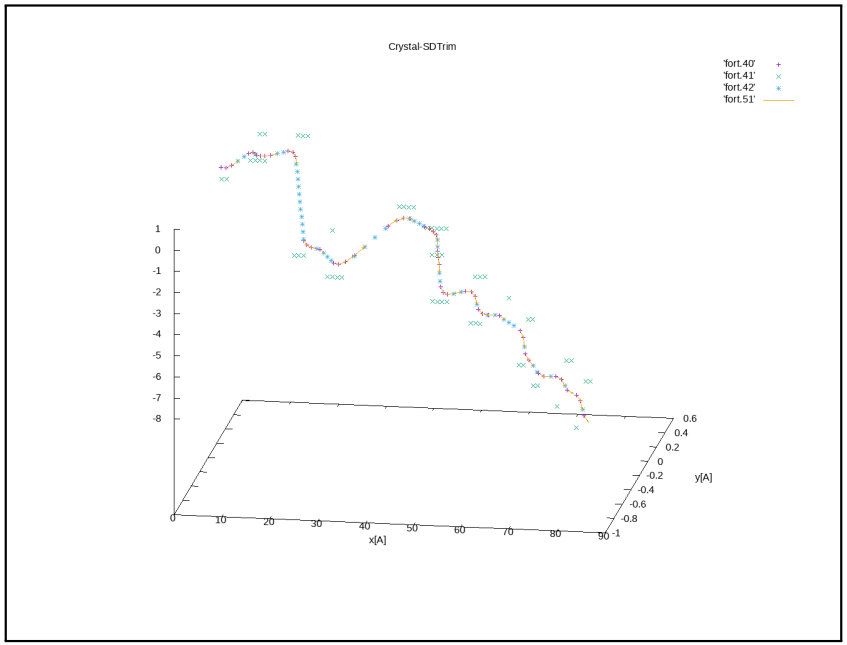


SDTrim not suited for modelling due to its assumption of amorphous atom distribution
Requires (too) expensive MD or e.g. MARLOWE (commercial, development stopped around 2000)

Modelling: Crystal-SDTrim

Development of Crystal-SDTrimSP: select next atom according to lattice structure

Lattice structure provided by basis-cell vectors and set of atom positions inside elementary cell



Reproduces experimental observations $\rightarrow$ will be included as option in SDTrimSP 6.08+