Applied Statistical Model of Surface Morphology for Plasma-Material Interactions

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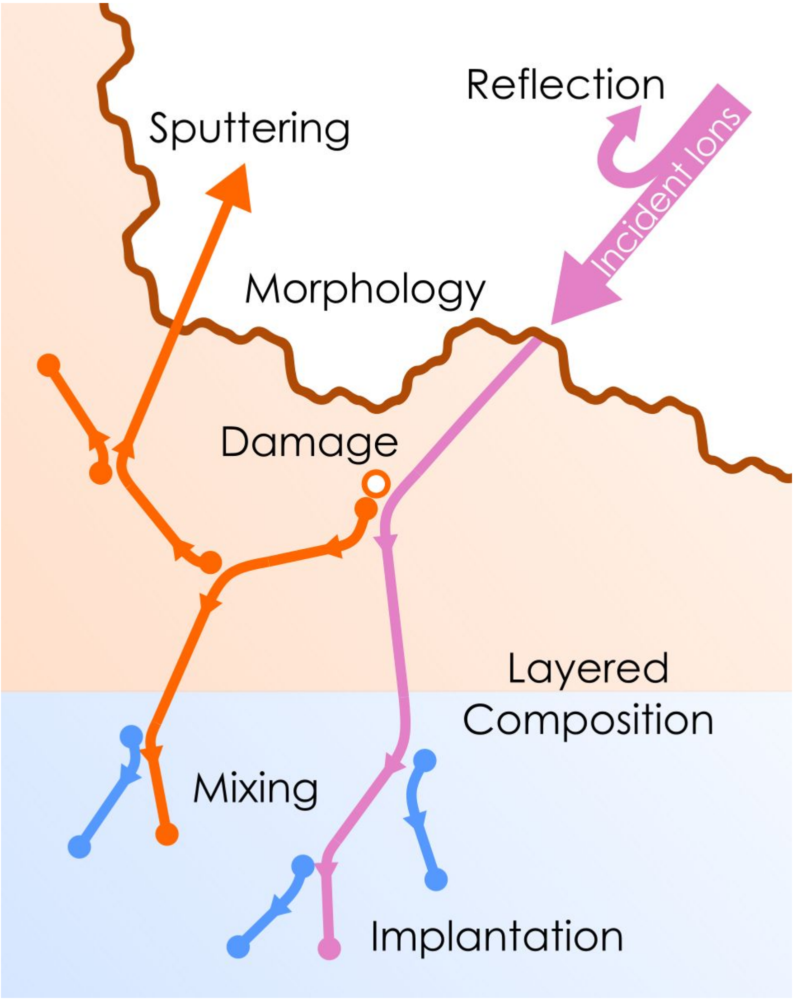
Fractal-TRIDYN (F-TRIDYN)



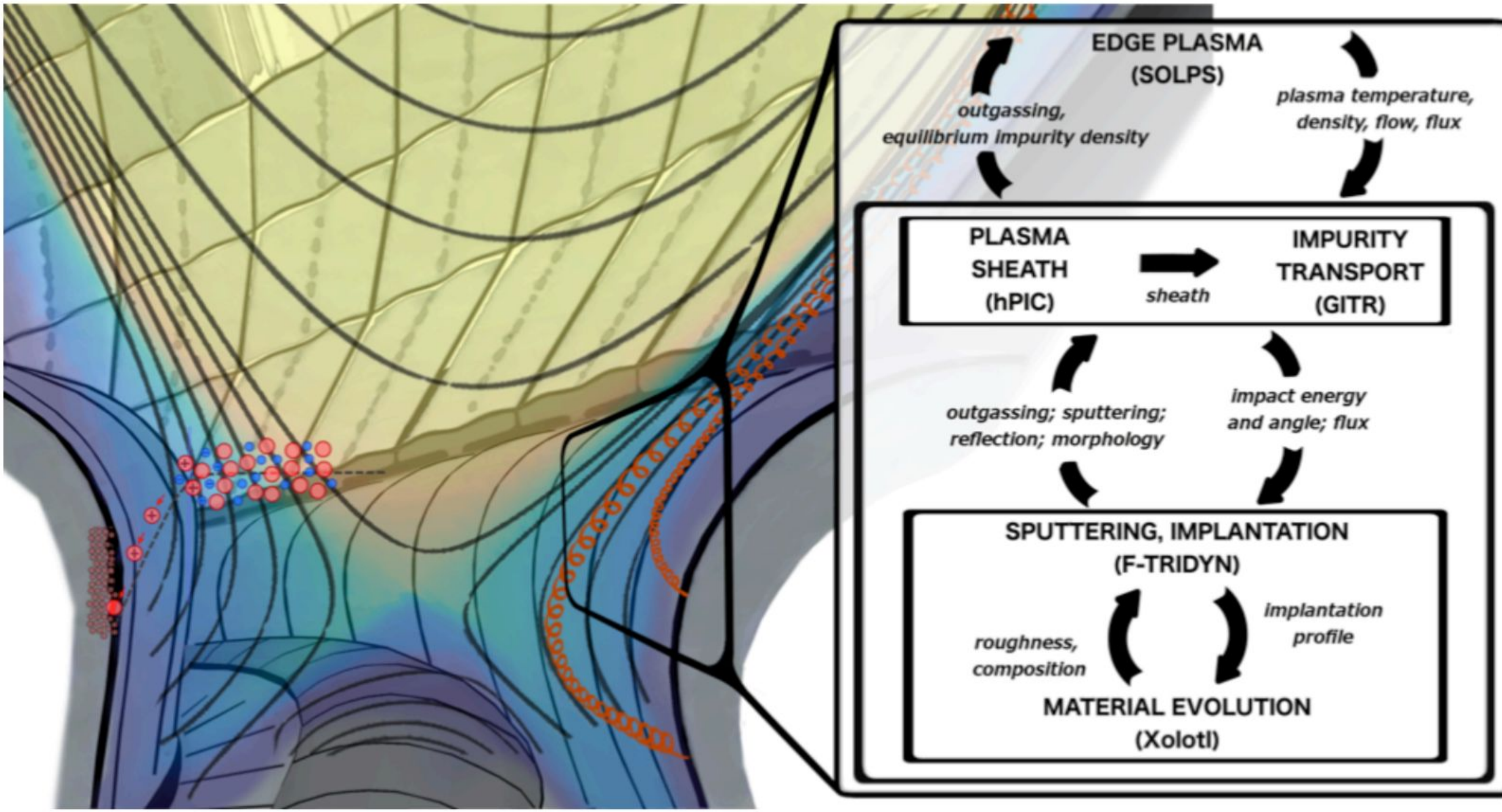
F-TRIDYN is a BCA code for ion-solid interactions

F-TRIDYN includes surface morphology:
- Fractal surface morphology
- Arbitrary polygonal surface morphology
- Statistical surface morphology

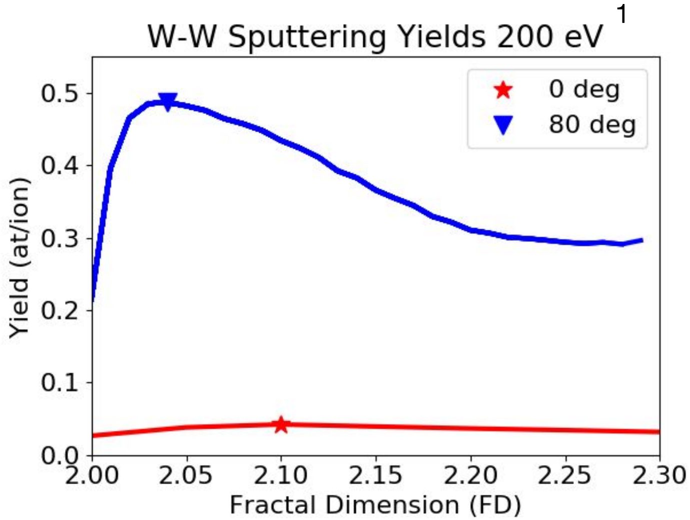
Computationally efficient model for:
- Reflection
- Sputtering
- Stopping
- Frenkel Pair Creation
- Mixing

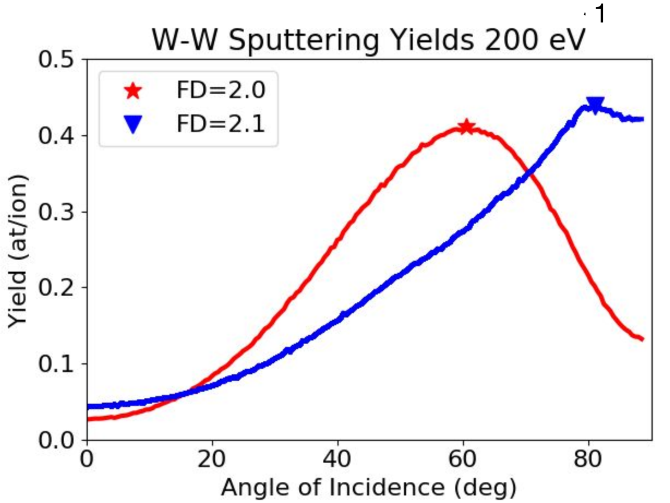
Output of relevant particle positions in 3D:
- Sputtered particle distributions
- Implanted particle positions
- Stopped PKA and SKA particle positions
- Damage profiles

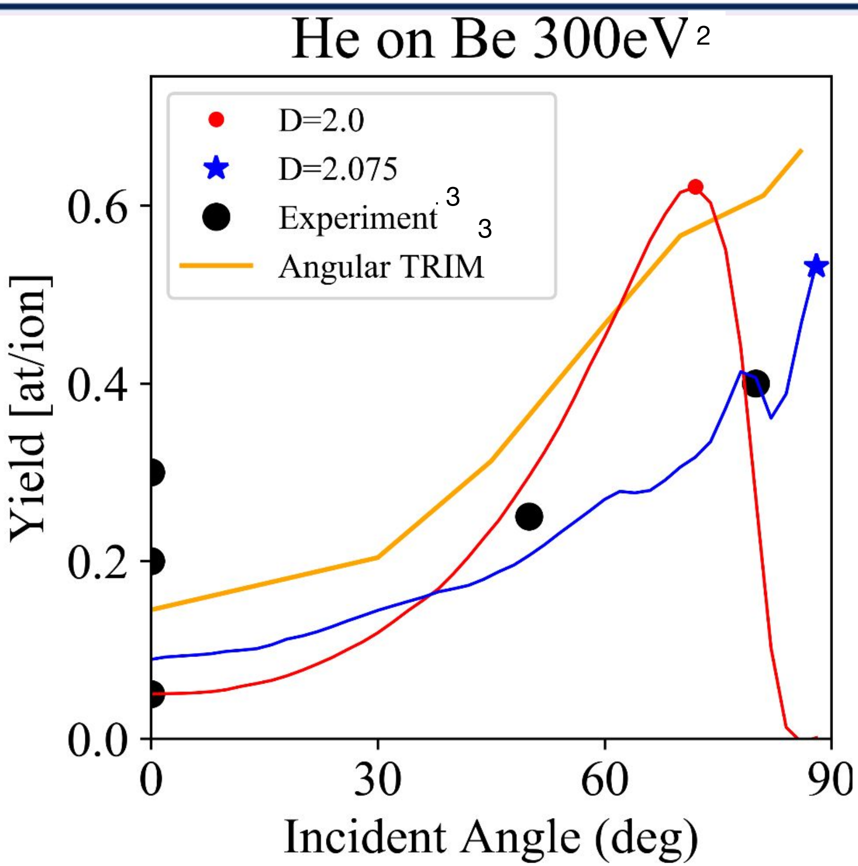
PSI-SciDAC 2 Project: Multiscale Modeling



Results: Sputtering Yield Curves with Fractal Surface Model







- Yield curves usable as rough surface response model
- Not feasible if there are many dynamic parameters
- Surface roughness shifts maximum yield to the right
- Little experimental sputtering yield data at low energies

[1]Drobny et al., 2018 [2]Drobny et al., 2016 [3]Küstner et al., 1999

Explicit versus Implicit Surface Models

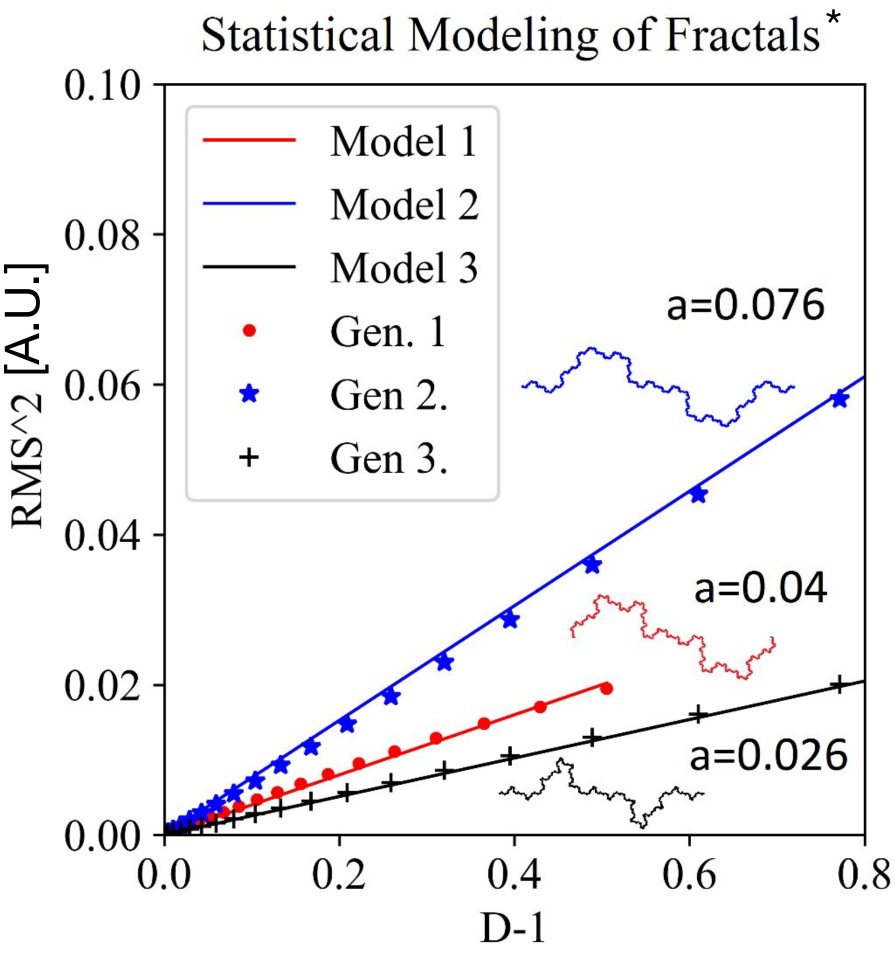
Fractal surface model

- Surface modeled as explicit fractal surface
- Fractal Dimension as roughness parameter
- Scale parameter also needed
- Surfaces created using fractal generators
- Requires additional scaling parameter
- Slow check of particle positions, O(n)
- Full capture of complex morphology
- Algorithm extendible to any 2D surface

Implicit, Statistical surface model

- Surface modeled as distribution of heights
- Single Gaussian model tied to RMS roughne
- Gaussian Mixture (N Gaussians) particularly suited
- Fast check of particle positions, O(N)
- Implicit structure only
- No spatial correlation captured

Link Between Fractal & Statistical Models

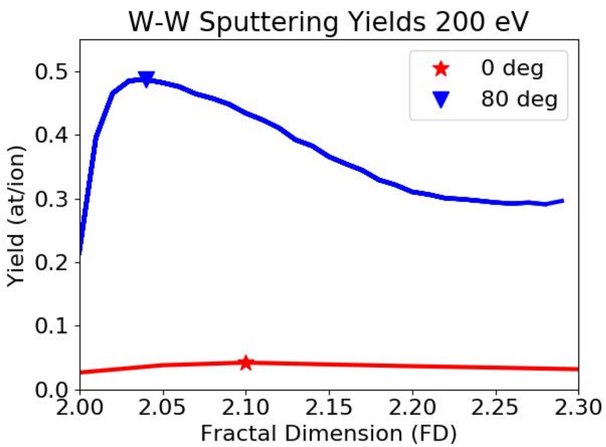


- Linear relationship between variance and D
- Holds for all tested fractal generators
- Allows a link between fractal and statistical models
- Reduces surface morphology to a single parameter
- Similar to (t)^(1/2) dependence of standard deviation of Brownian motion

*Drobny et al., 2016

Sputtering Yields with Single Gaussian Surface Model

Fractal Model

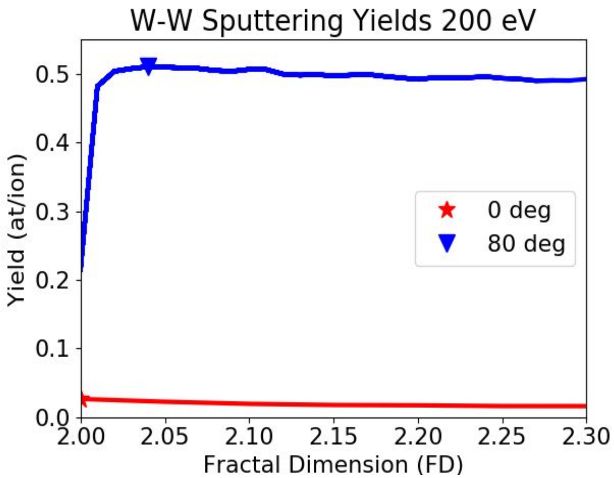


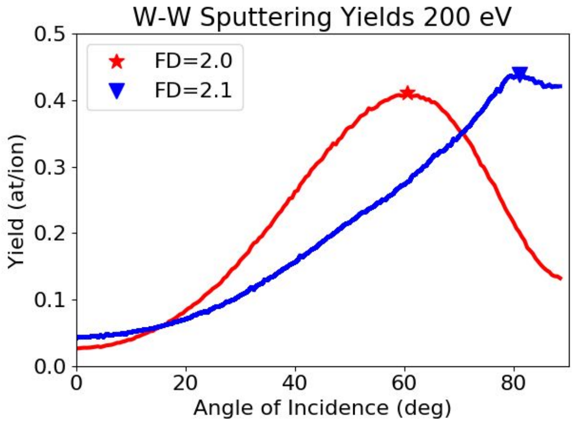
Single Gaussian surface model only captures low-roughness behavior of complex fractal surface

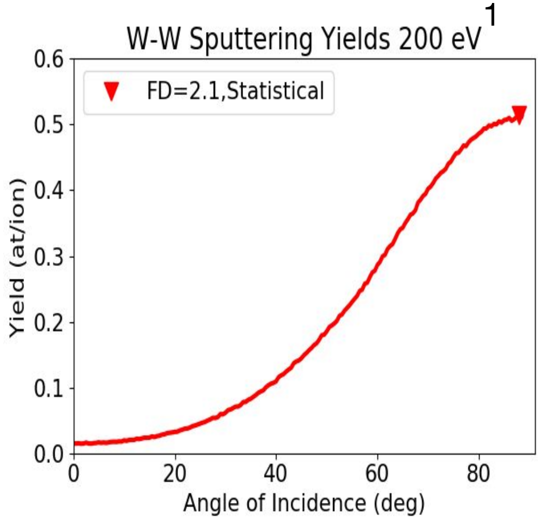
Saturation of yield with increasing surface roughness observed qualitatively in experiments

Single Gaussian surface model describes a surface without complex structure, resulting in the step-like behavior of sputtering yield

Statistical Model with 1 Gaussian

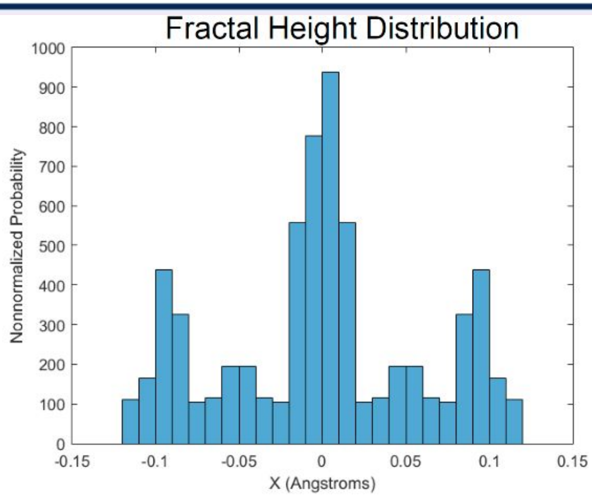


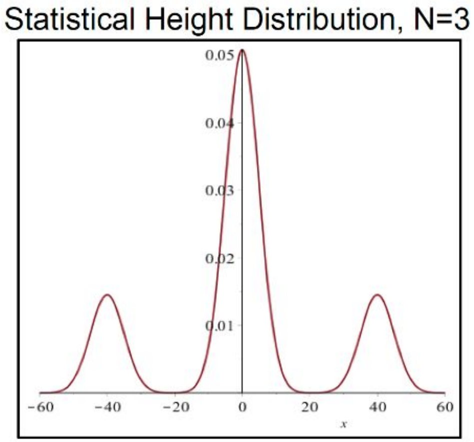




[1]Drobny et al., 2018

Beyond The Normal Distribution: Gaussian Mixture Model





Gaussian mixture model, fitted to surface height distributions, can capture more complex surfaces than a single Gaussian peak.

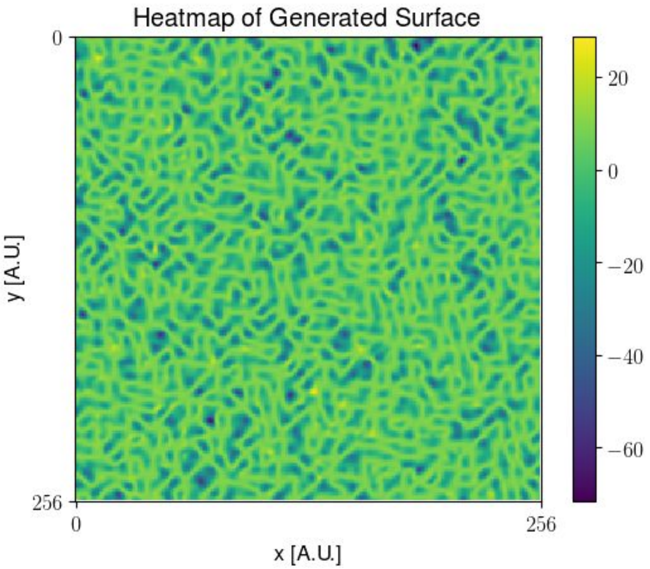
PDF:

$$f(x) = \sum_{i=1}^{N} \frac{W_i}{\sqrt{2 \cdot \pi \cdot \sigma_i}} \cdot \exp\left\{ -\left(\frac{x - \mu_i}{\sqrt{2}\, \sigma_i} \right)^2 \right\}$$

CDF:

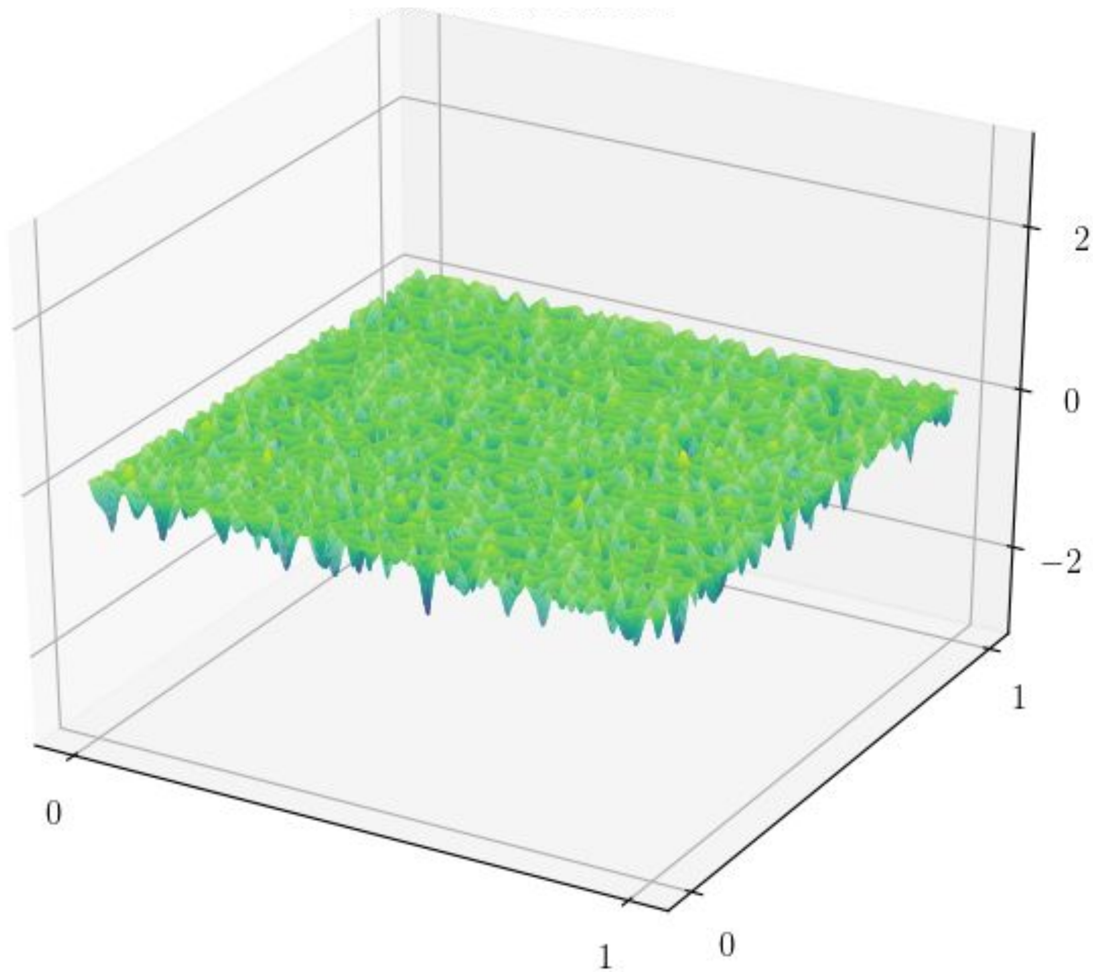
$$g(x) = \int_{-\infty}^{x} f(x')\,dx' = \sum_{i=1}^{N} \frac{W_i}{2} \left(1 + \operatorname{erf}\left\{ \frac{x' - \mu_i}{\sqrt{2}\, \sigma_i} \right\} \right)$$

Generated Surfaces for Testing



A Gaussian mixture model allows for the fast modeling of realistic surfaces.

This surface was created via combination of multiple layers of simplex noise.

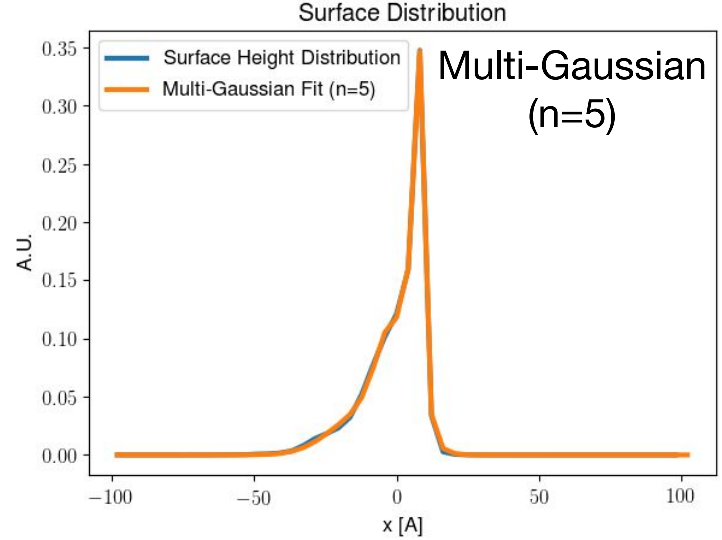


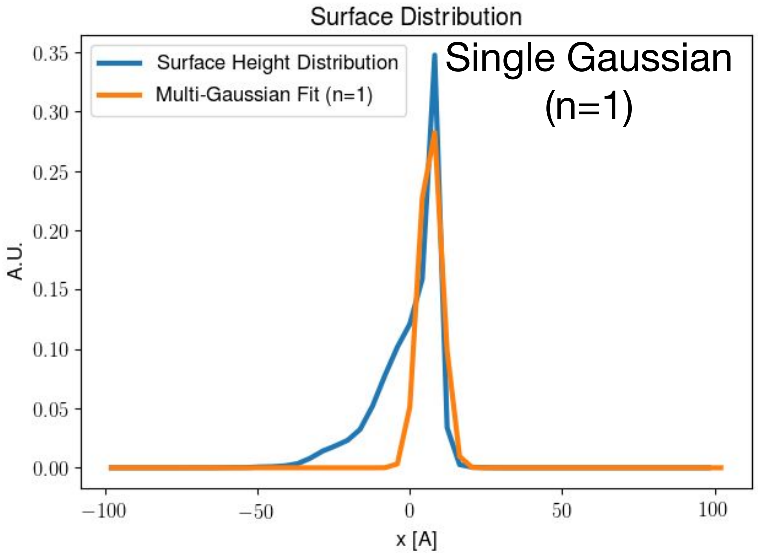
Statistical Modeling of Generated Surfaces

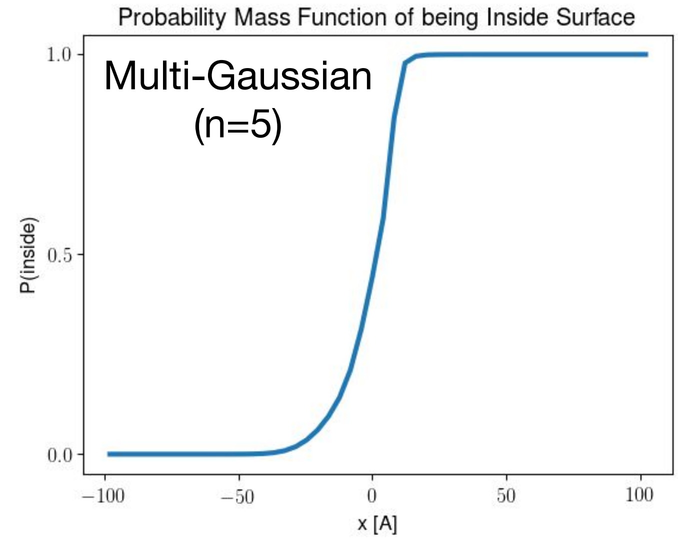
An optimization routine was used to fit the Gaussian Mixture Model to the surface height distributions.

A single Gaussian peak (below) cannot model the generated surface. The surface was scaled up by a factor of 100 for use in the BCA.

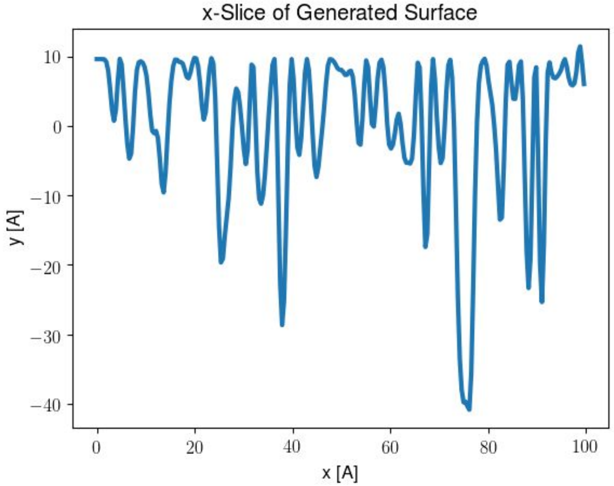
Instead, 5 Gaussians can reproduce the surface height distribution (above right) and the corresponding CDF (below right) (PMF of being inside the surface at a given depth) with ease.



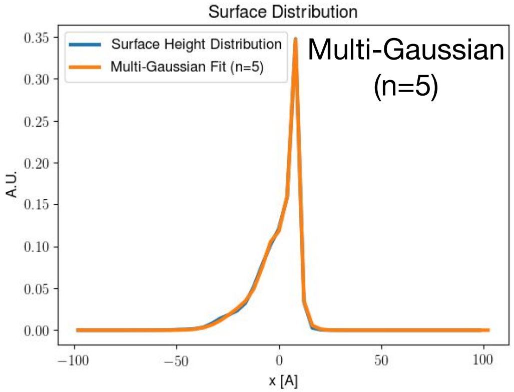


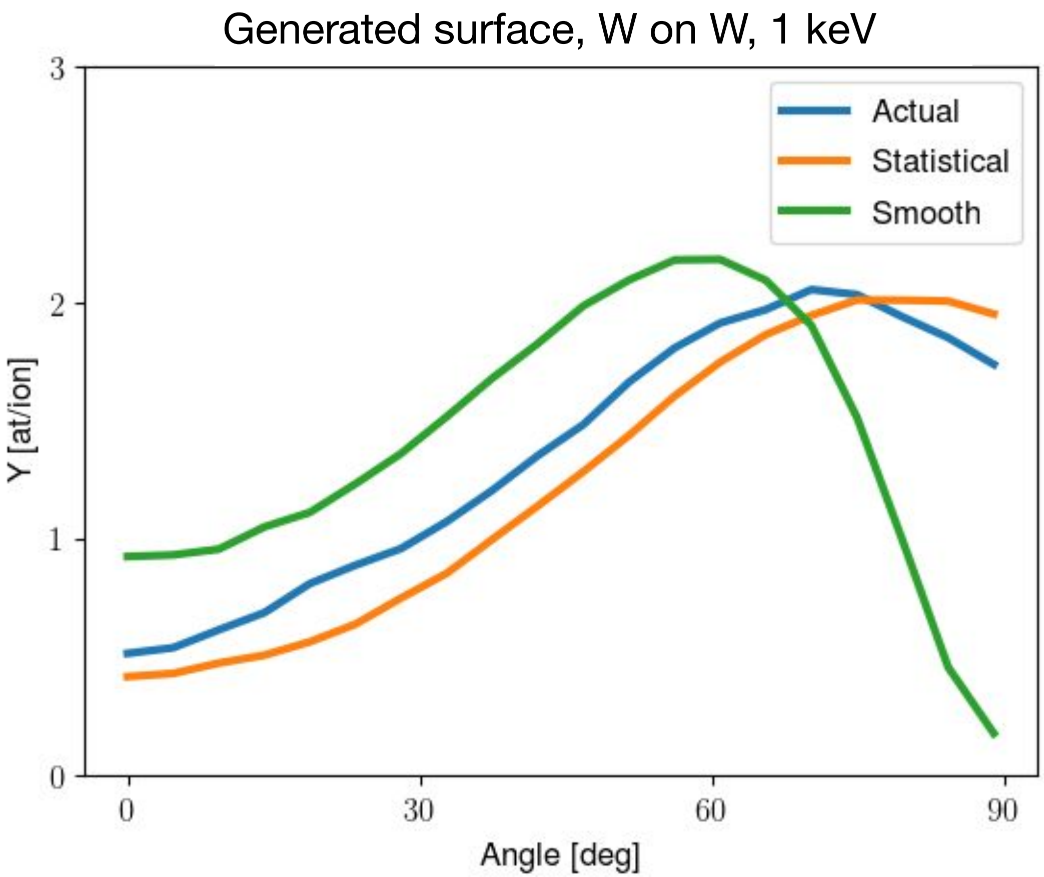


Generated Surface Sputtering

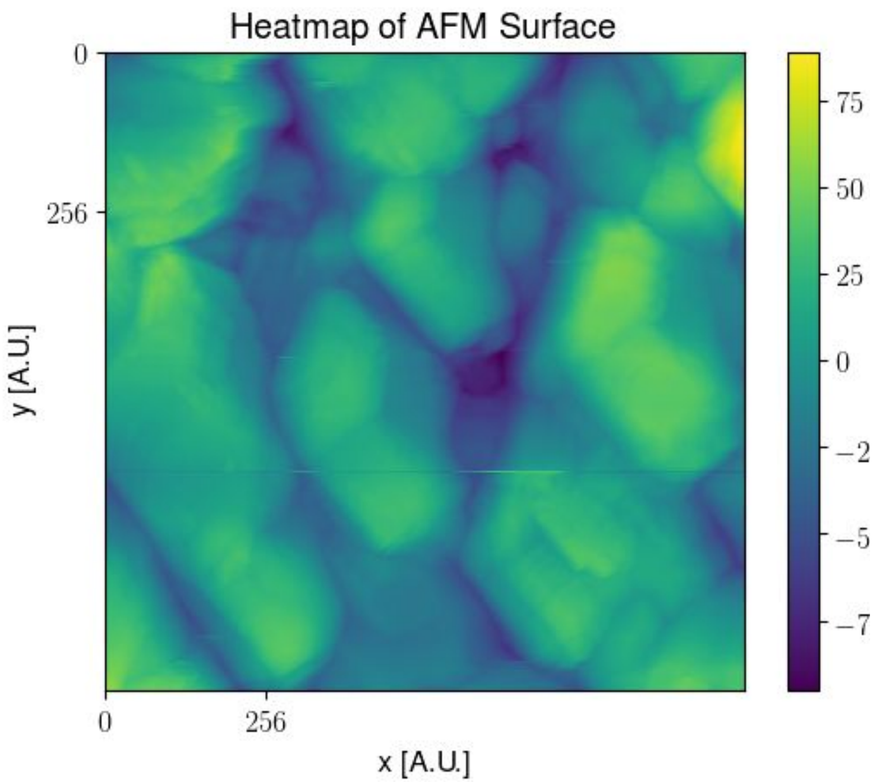


Using the above surface slice to represent the surface in 2D and the below statistical model, the sputtering yield versus angle can be found.

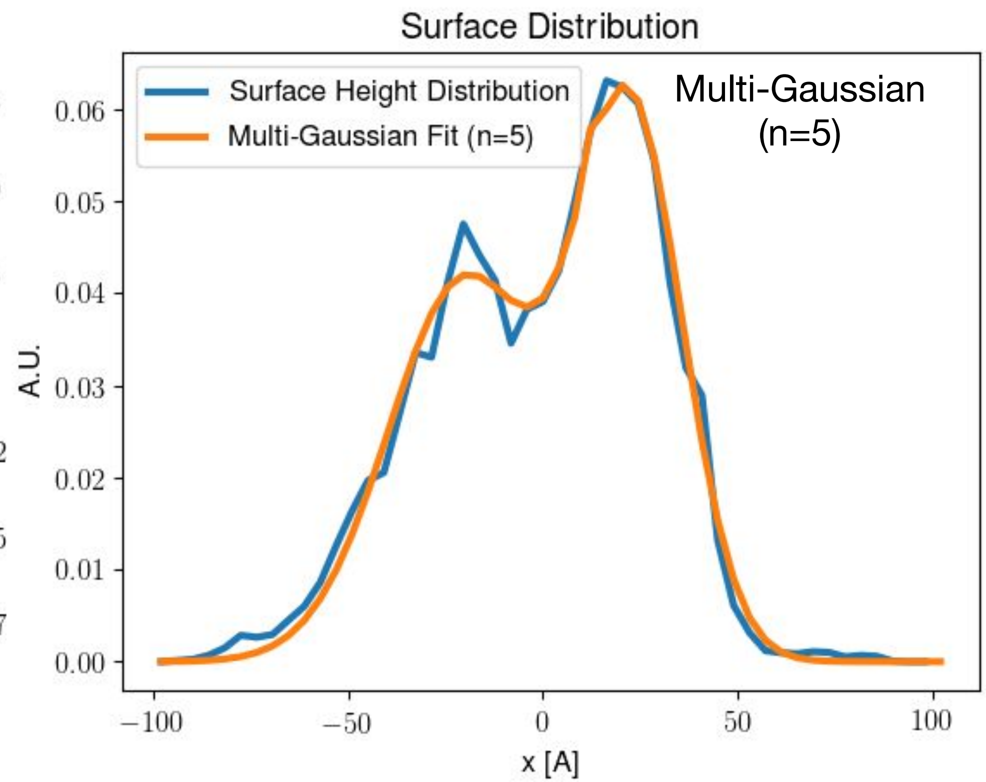




AFM Surface: Porous Tungsten

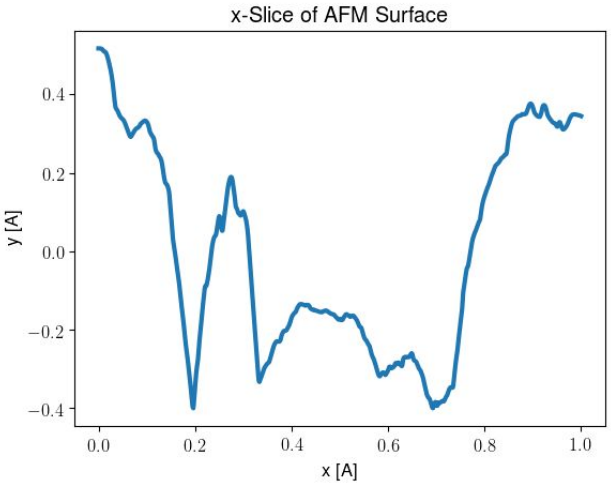


Instead of using generated surfaces, the same model works for surfaces generated from AFM images. This is a test AFM image of porous, sintered tungsten.



The corresponding surface height distribution and the fit for an N=5 Gaussian-Mixture Model.

AFM Surface Results



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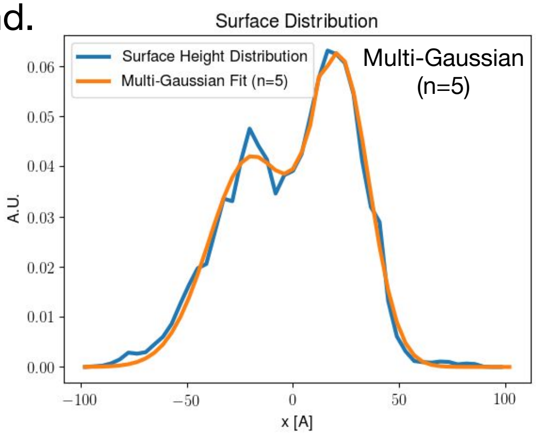
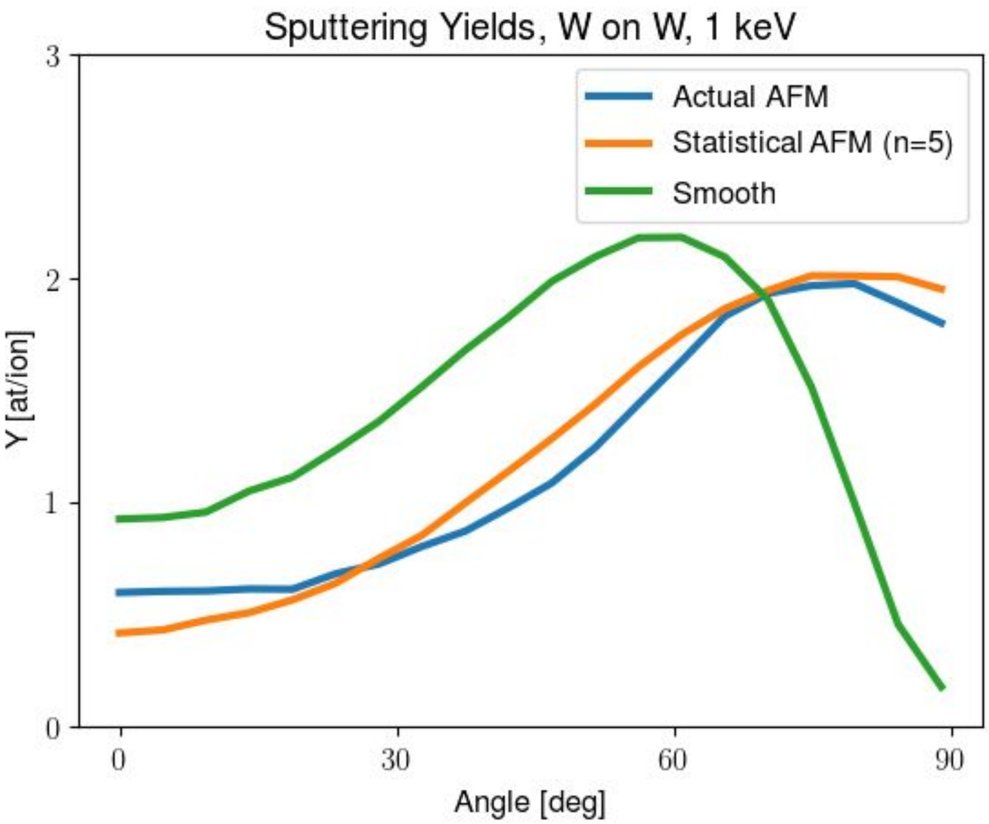




Future Work

Additional upgrades to statistical model include:

- Spatial dependence of surface parameters
- Larger surface features present problems

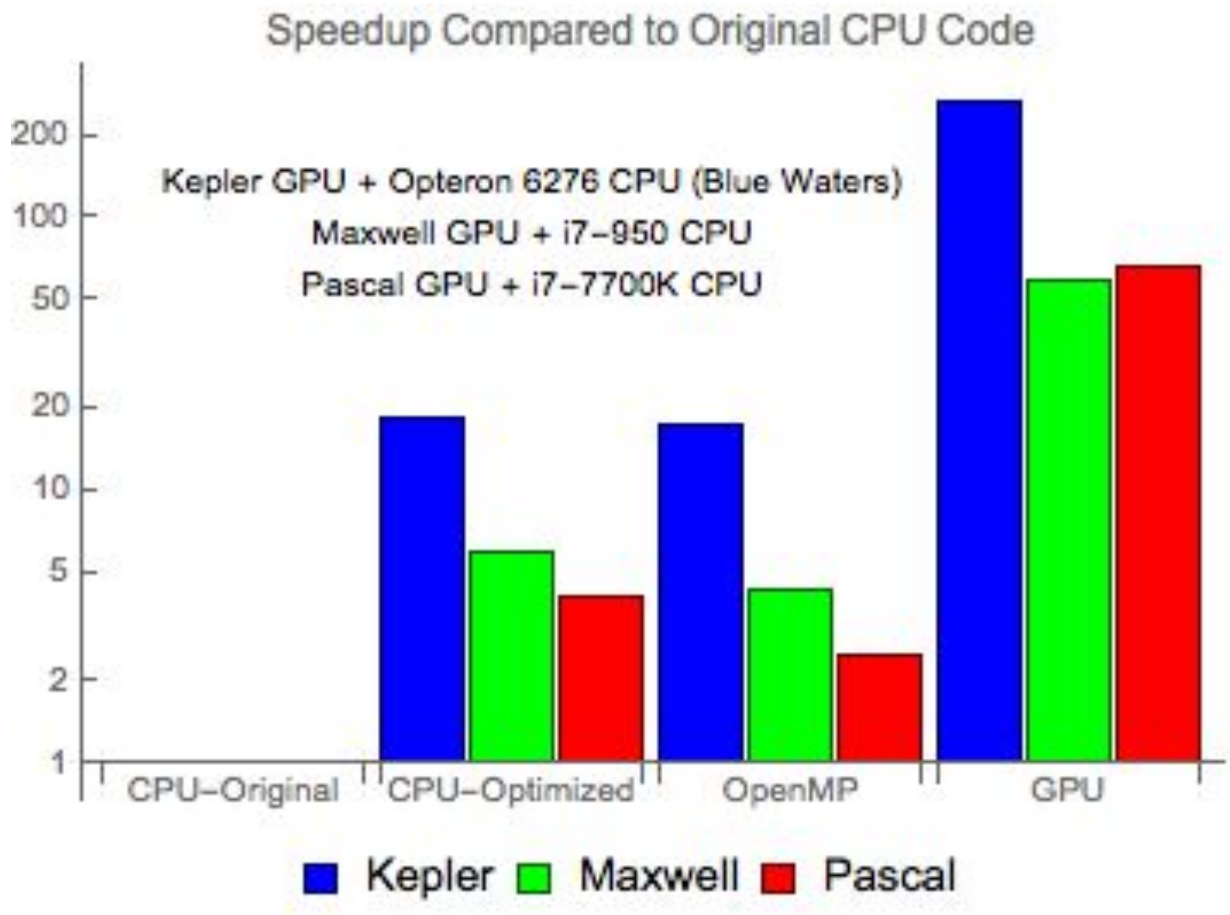
Further verification/validation

- Next step: comparison to experimental surface
- Measuring sputtering yield of real, rough targets

OpenBCA

- New Binary Collision Approximation code for ions and more
- Written in modern syntax C
- Massively parallelizable on CPUs and GPUs
- Planned to be open source addition to available plasma physics codes
- Designed with in-memory code coupling in mind
- Plans for implementation of mesh-based geometry including spatially dependent composition
- Primary Developer: **Kurt Gimbel**

Parallelization: CUDA, OpenMPI



Speedup with parallelization is substantial with the prototype code.

Additional Physics and Features

Flexibility in:

- stopping power formulation
  - Currently implemented:
    - Lindhard-Scharff (low-energy)
    - Bethe-Bloch (high-energy)
- particle-particle interaction potential

Target composition pulled from other codes to include more physics (e.g., Xolotl)

Includes same surface models present in F-TRIDYN (explicit polygonal morphology and statistical surface model)

Future plans for meshed 3D geometry at both micro- and macroscopic scales

Open Source

Many BCA codes are closed source or limited access

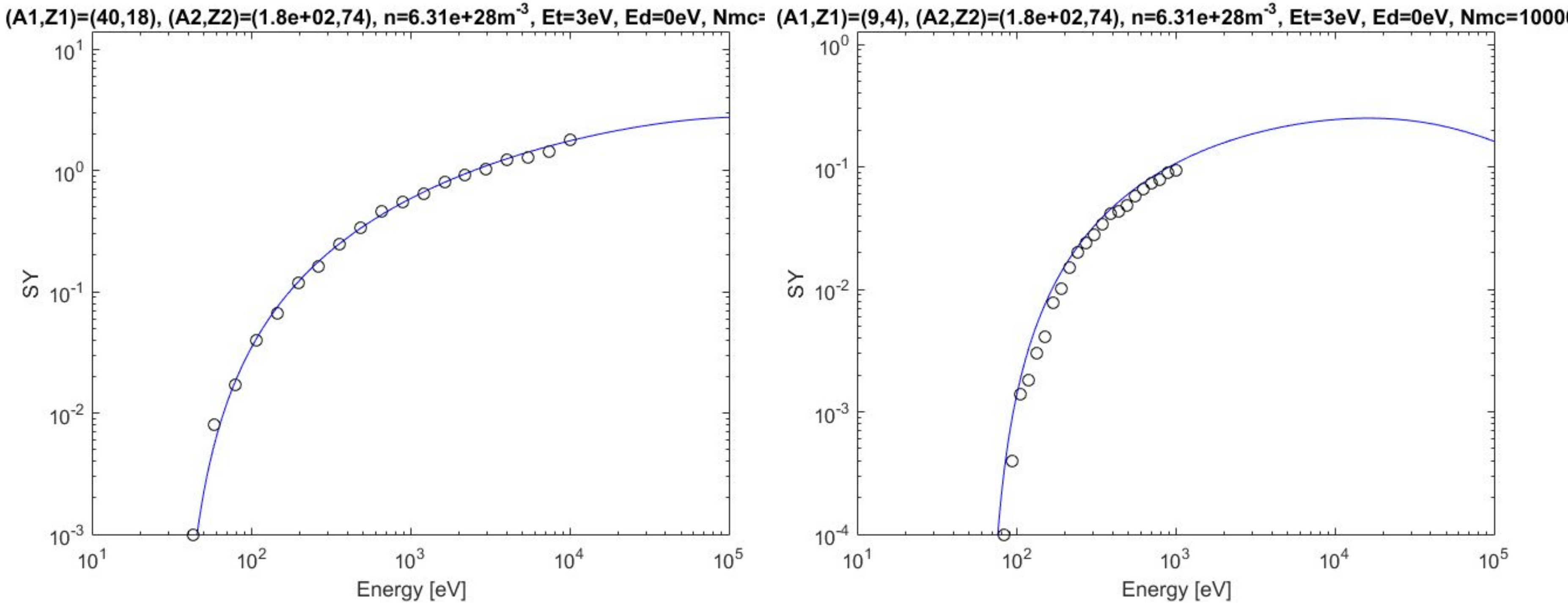
SRIM is free to download and widely used

Issues with SRIM results with difficult to diagnose causes:

- Effect of deep particle start condition[3]
- Significant overestimation of light ion sputtering[3]
- Incorrect sputtered particle angular distributions[4]

SRIM is closed source – problems with this widely used code are either of unknown cause or inferred cause

Validation Against Empirical Formulas



Comparison to Yamamura semi-empirical sputtering formula shows promising results.

Currently, OpenBCA reproduces TRIDYN results down to the sputtering threshold and far includes the statistical surface model as presented in this talk

Conclusions and Future Work: OpenBCA

OpenBCA is a promising framework for simulation and integration into coupled codes of ion-material interactions

The BCA is well-suited to parallelization, and the OpenBCA prototype is already scaling well on high performance computers

Further development of the code

Verification and Validation versus experiment and older, well-verified BCA codes

Implementation of new features, including additional physics and code coupling interfaces

Improving parallelization scheme

References and Acknowledgements

[1]Drobny et al., both papers

[2] Küstner et al., Journal of Nuclear Materials 265 (1999) 22-27

[3]V.I. Shulga, Note on the artefacts in SRIM simulation of sputtering, Applied Surface Science 439 (2018) 456-461

[4]H. Höfsass, et al., Simulation of ion beam sputtering with SDTrimSP, TRIDYN and SRIM, Applied Surface Science 15 (2014) 134-141

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