Fast, Statistical Model of Surface Roughness for Ion-Solid Interaction Simulations and Efficient Code Coupling

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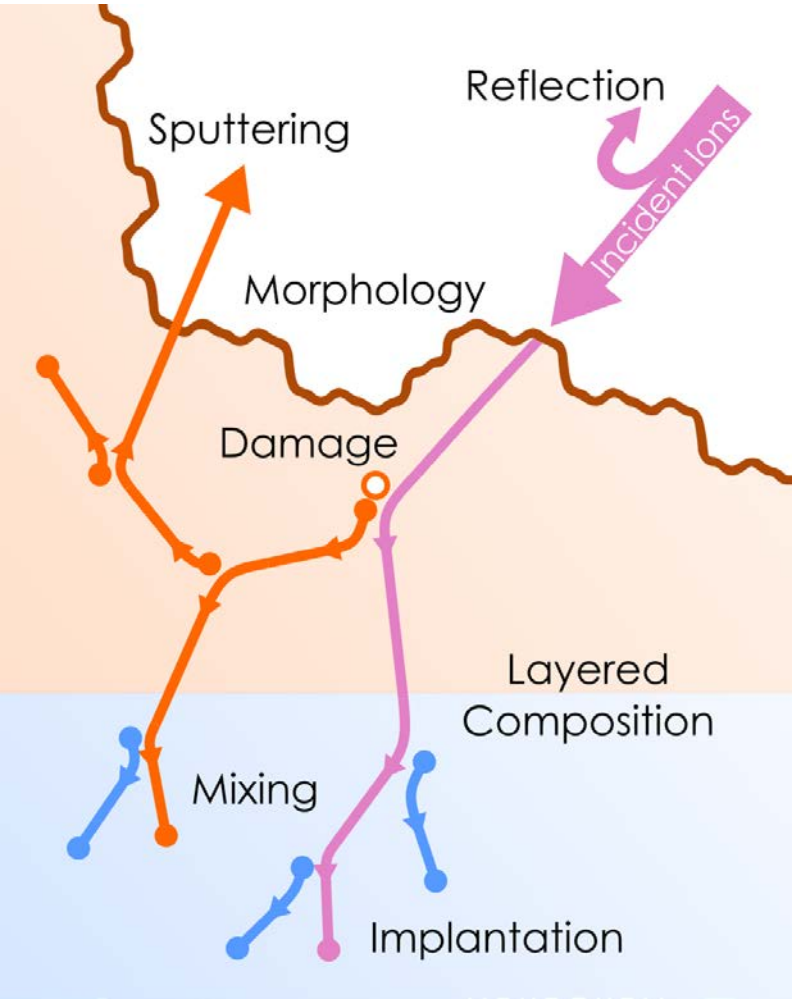
Fractal-TRIDYN (F-TRIDYN)



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

F-TRIDYN includes surface morphology:
- Fractal surface morphology
- 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
- Frenkel Pair creation positions

Motivation: BCA for Coupling

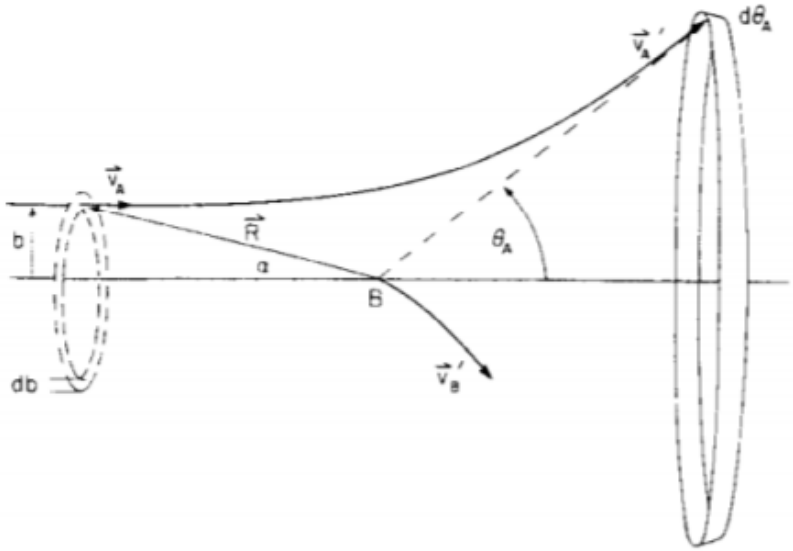
Binary Collision Approximation (BCA) codes handle atomic timescale (ps-fs) and lengthscale (Å-nm) ion-solid interactions

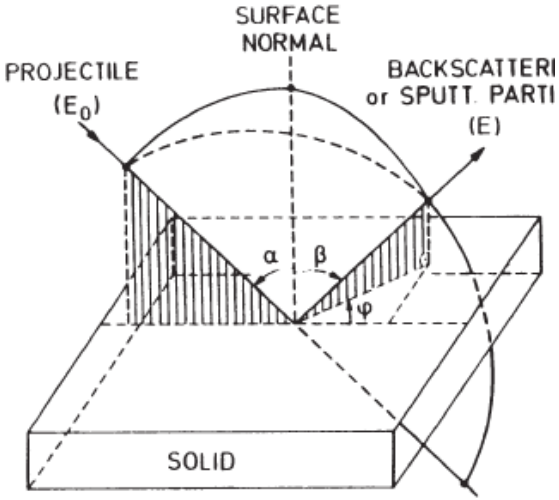
Significantly faster than Molecular Dynamics for ion-solid interactions

Dynamic materials have too many free parameters to capture using empirical or analytical formulas

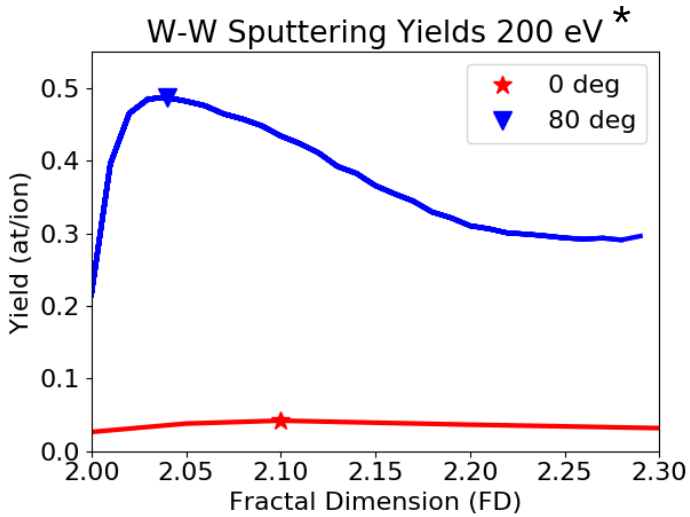
Physics captured using binary nuclear collisions and a formula for electronic stopping

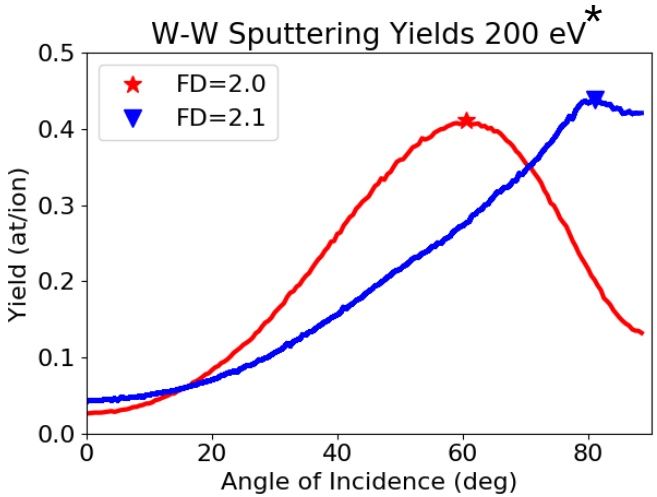
BCA codes have been verified for many systems for decades

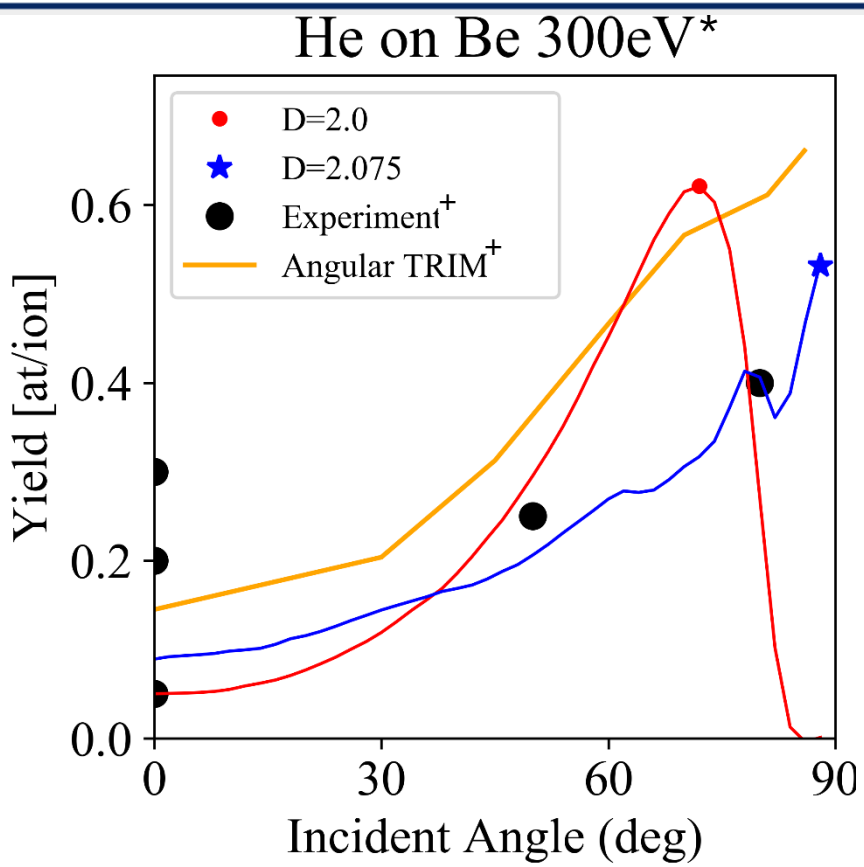




Results: Sputtering Yield Curves with Fractal Surface Model





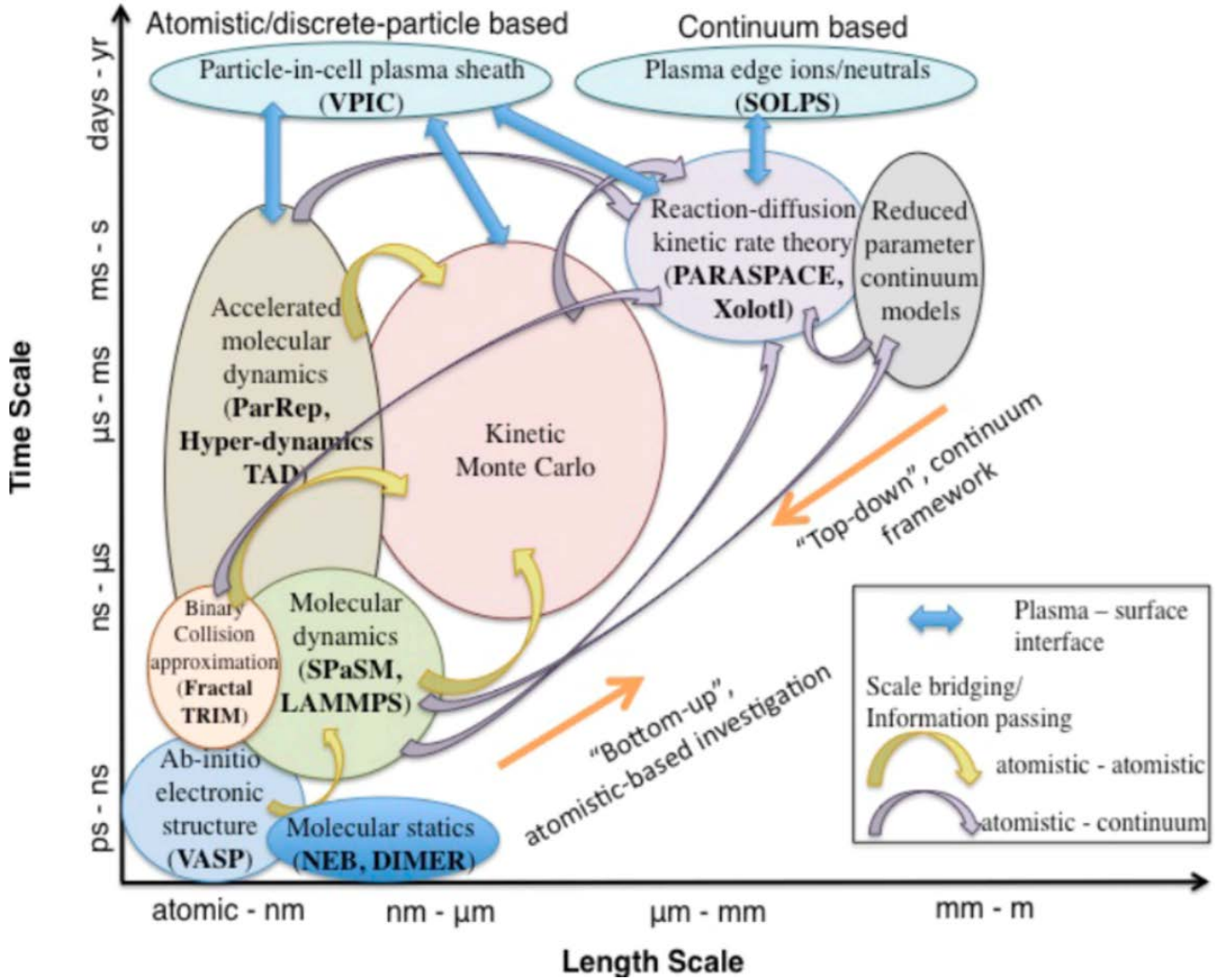


- Yield curves usable as rough surface response model
- Not feasible if there are many dynamic parameters
- Surface roughness shifts maximum yield to the right
- Little experimental sputtering yield data at low energies

*Drobny et al., 2016

+Küstner et al., 1999

PSI-SciDAC 2 Project: Multiscale Modeling

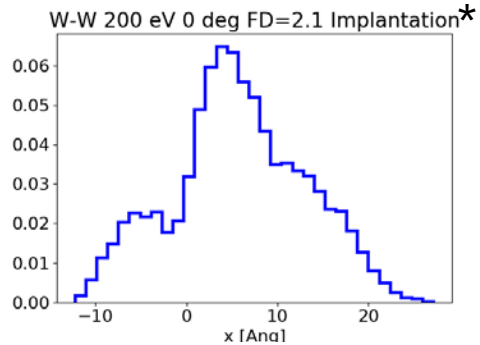


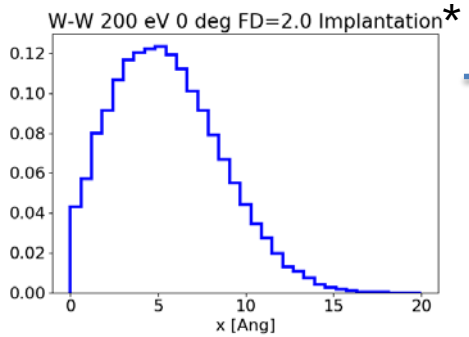
Code Coupling: Applications

Ion Energy
Ion Angle
Material Properties
Surface Morphology
Target Composition

F-TRIDYN

Implantation Distributions

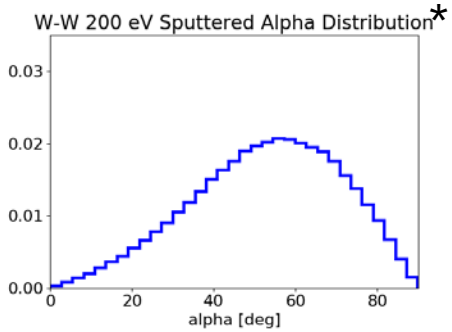


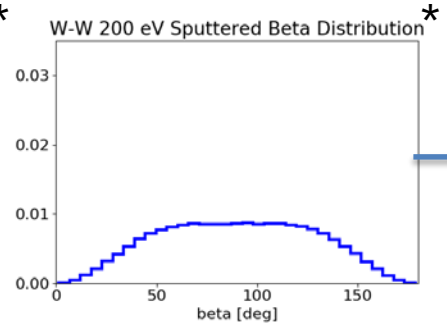


Material (Xolotl)

Surface Evolution
Effect on Plasma

Sputtered Atom Distributions





Plasma (GITR,hPIC)

*Drobny and Curreli (submitted)

Theory: Surface Roughness 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 (~100s)
- Full capture of complex morphology
- Algorithm extendible to any 2D surface

Statistical surface model

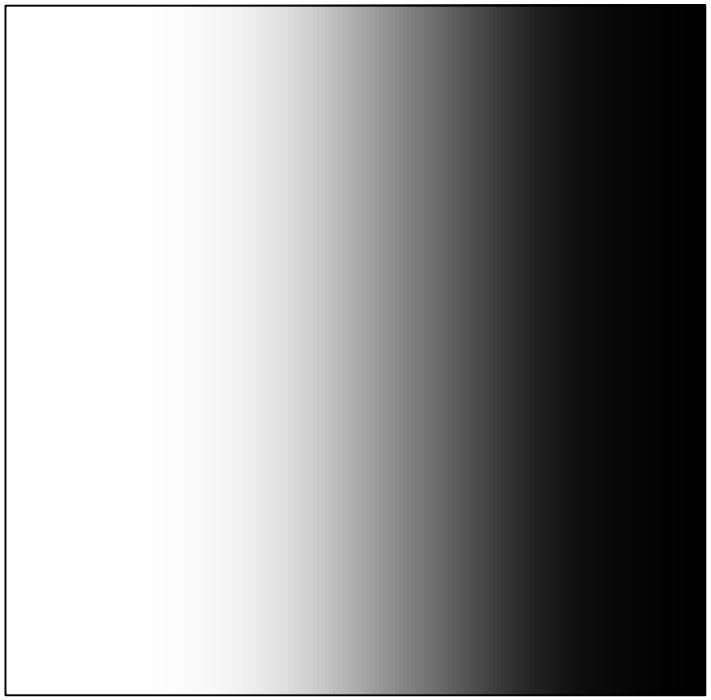
- Surface modeled as distribution of heights
- RMS roughness as roughness parameter
- Standard measure of surface roughness
- Fast check of particle positions (~10s)
- Up to 50X faster than explicit surface
- Implicit structure only
- No spatial correlation captured

Theory: Normally Distributed Surface Heights

Assume normally distributed surface heights

Probability of a given position being inside the surface is given by the error function

Not a CDF, but a Probability Mass Function (PMF)
Same functional form as CDF for normal distribution

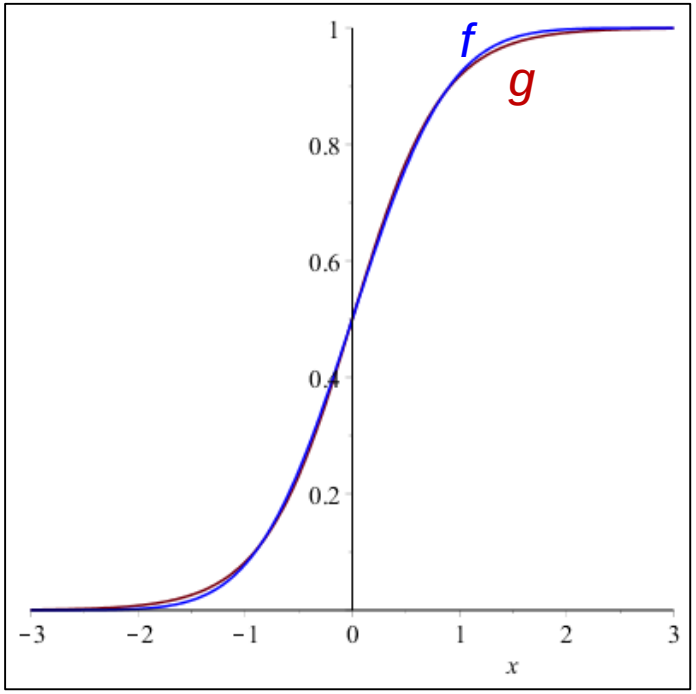


Logistic approximation to erf() for whole domain

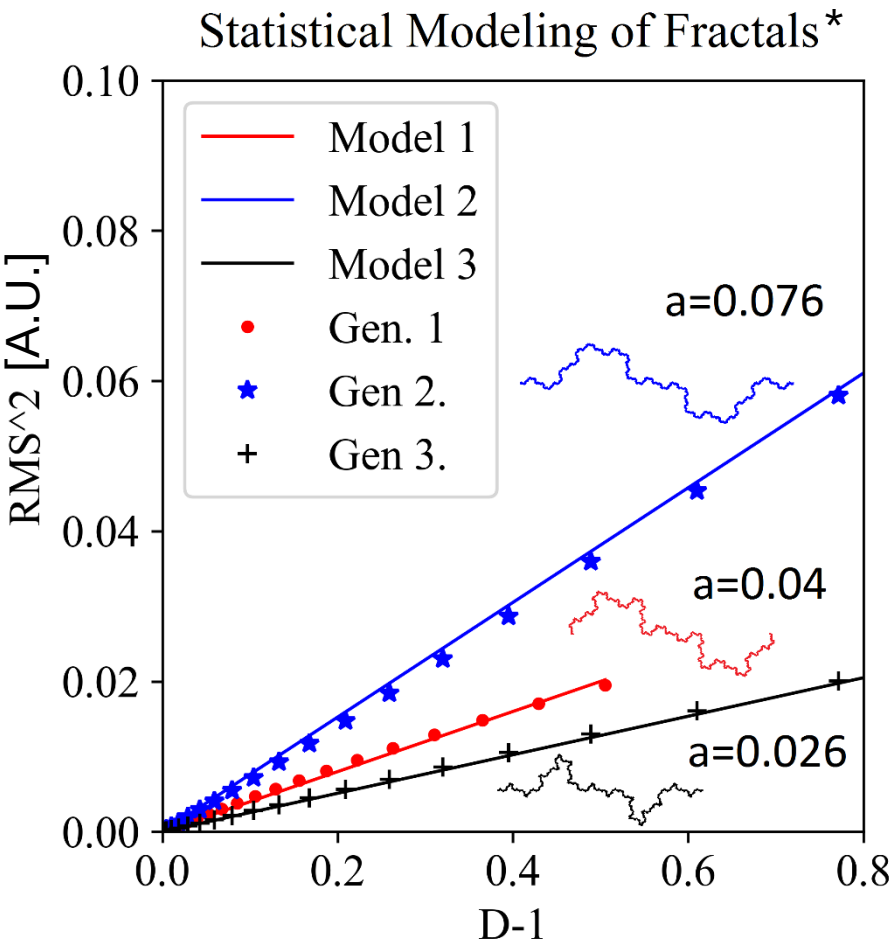
Minimizing total square error leads to a=1.70/σ*

Logistic function is invertible and analytic

$$f = \frac{1}{2} - \frac{1}{2}\mathrm{erf}\left(\frac{x}{\sqrt{2}\,\sigma}\right) \qquad g = \frac{1}{1 + \exp(-a\,x)}$$



Theory: Link Between Fractal & Statistical Models

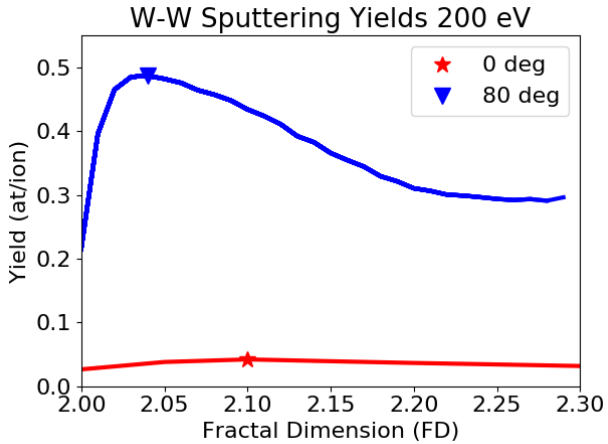


- Linear relationship between variance and D
- Holds for all tested fractal generators
- Allows a link between fractal and statistical models
- Reduces surface morphology to a single parameter
- Similar to (t)^(1/2) dependence of standard deviation of Brownian motion

*Drobny et al., 2016

Initial Results: Sputtering Yields with Statistical Surface Model

Fractal Model*



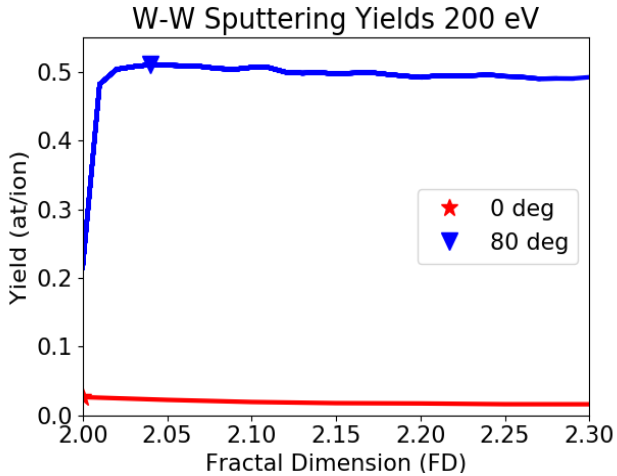
Single Gaussian surface model only captures low-roughness behavior of complex fractal surface

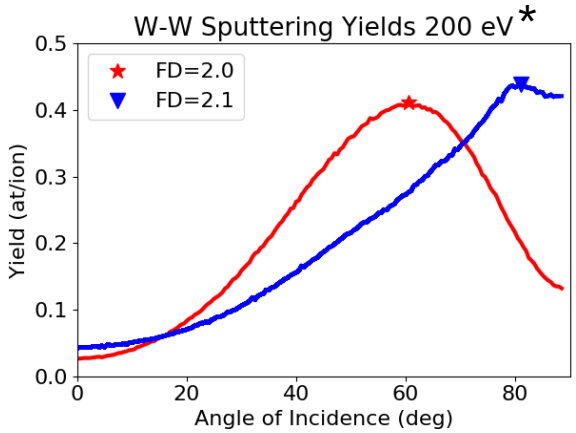
Saturation of yield with increasing surface roughness observed qualitatively in experiments

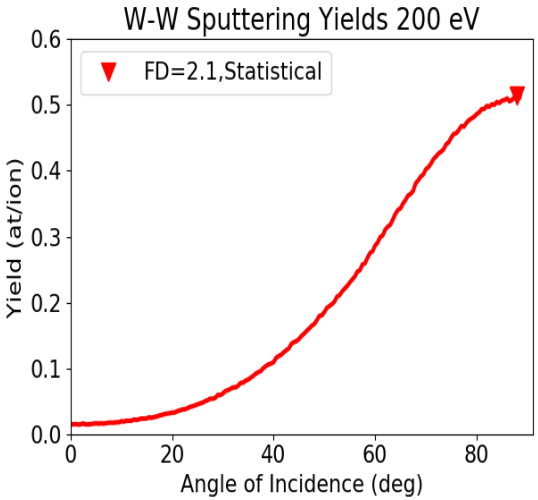
Statistical surface model describes a surface without complex structure, resulting in the step-like behavior of sputtering yield

Nonlinear relationship between FD and RMS roughness

Statistical Model

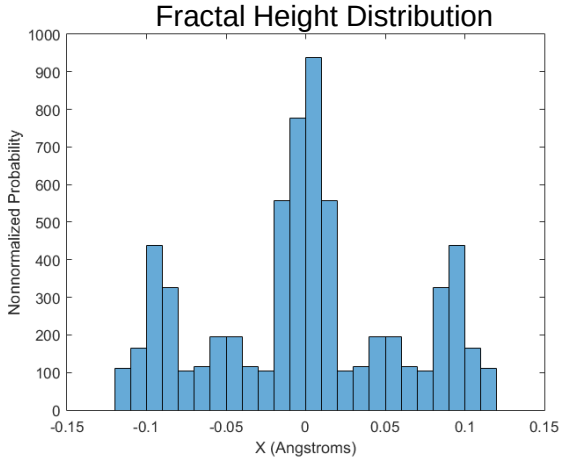


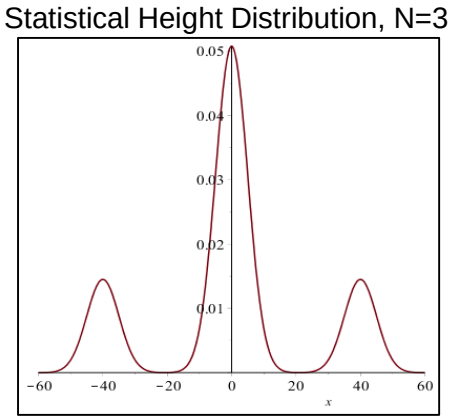


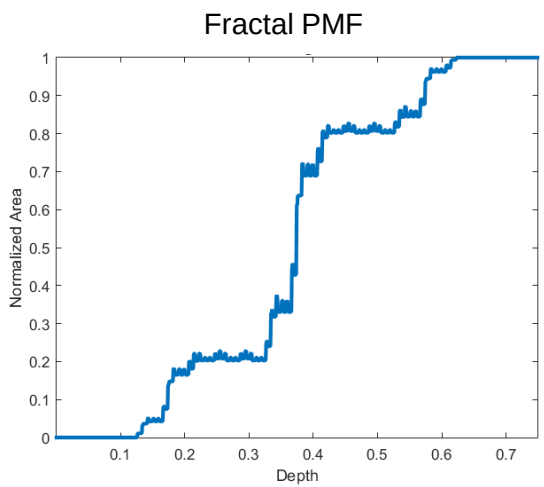


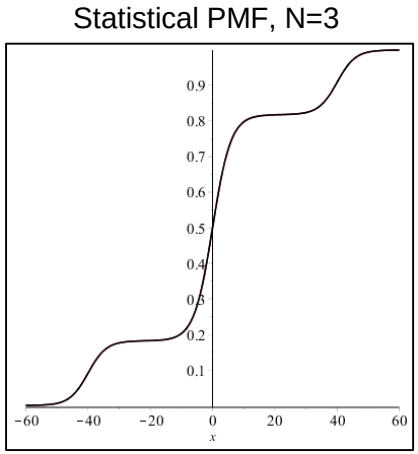
*Drobny et al., 2016

Modeling: Further Statistical Modeling of Complex Surfaces









Multi-Gaussian estimation

PMF now sum of kernels

Opens up possibility of directly modeling surface morphology from AFM measurements or other atomic scale imaging

Increase in computational cost is negligible

Kernel Density Estimation may be used to find PMFs of real surfaces

Conclusions

- A statistical model of surface roughness has been included in F-TRIDYN for ion-solid interactions
- Reduces surface roughness problem to a single parameter, the RMS roughness
- Approximate statistical structure of complex surface morphologies reproducible via kernel density estimation of surface height distributions

Future Work

- Pursuit of direct comparison to experiment using KDE technique to reproduce statistical properties of complex surface morphologies
- Investigation into possible additions or improvements to the BCA model of ion-solid interactions
- Improved code-coupling behavior for multi-scale modeling

References

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