A Two-Dimensional Lorentzian Distribution for an Atomic Force Microscopy Simulator

Lado Filipovic and Siegfried Selberherr

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Christian Doppler Laboratory for Reliability Issues in Microelectronics
Institute for Microelectronics, TU Vienna
Gußhausstraße 27–29, A-1040 Wien, Austria
Technische Universität Wien, Austria
http://www.iue.tuwien.ac.at

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- AFM Oxidation Kinetics

Modeling Oxidation Kinetics

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- Algorithm for the Gaussian Model
- Algorithm for the Lorentzian Model
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Introduction - Atomic Force Microscopy (AFM)

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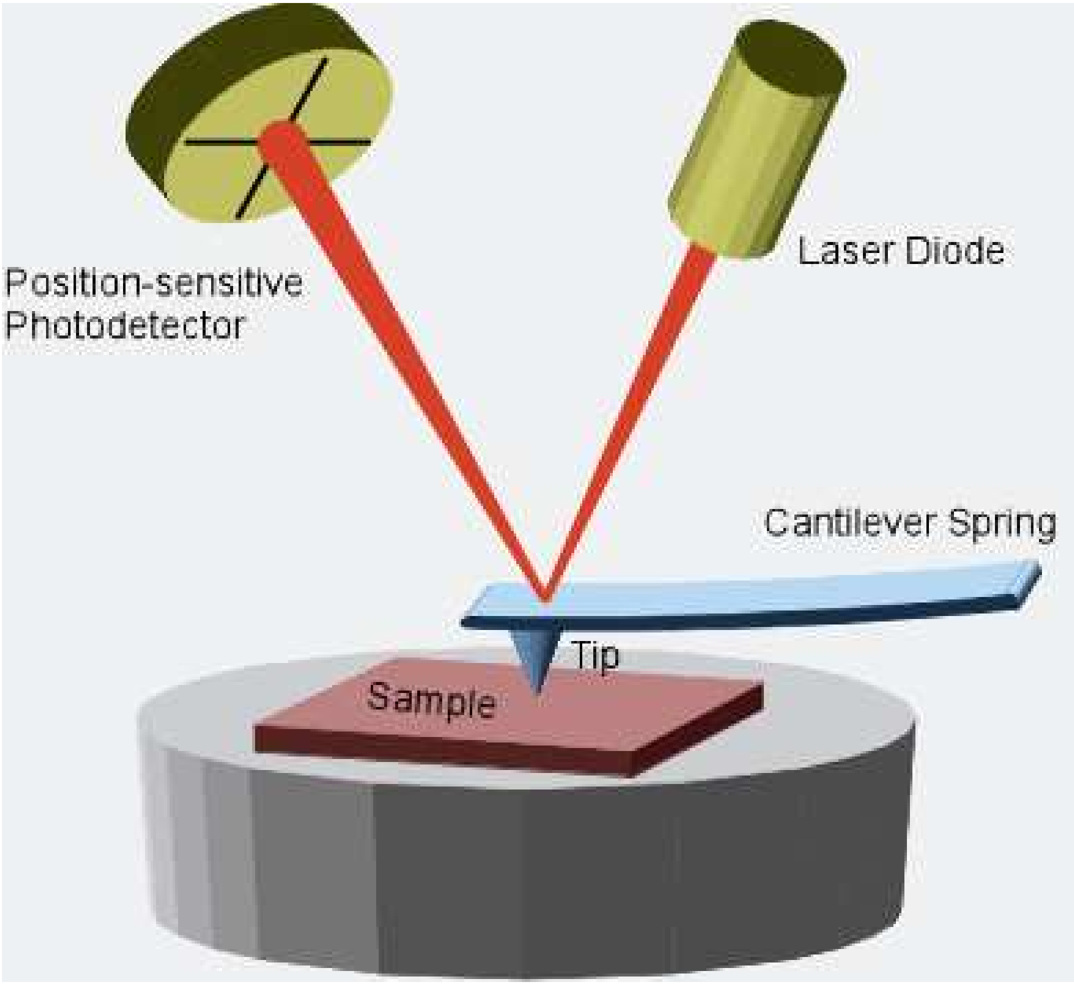
- Patterning tool for the deposition, removal, and modification of material surfaces with nanoscale precision.

Atomic Force Microscope



http://www3.physik.uni-greifswald.de/method/afm/eafm.htm

AFM Nanodot Oxidation Model

- AFM developed in 1986 by G. Binning, C.F. Quate, and C. Gerber
- Model for NC-AFM from Calleja [a] is implemented in the simulator.
- Equation governing oxide growth: $h(t,V) = h_0(V) + h_1(V)\ln(t)$
  $h_0(V) = -2.1 + 0.5V - 0.006V^2$
  $h_1(V) = 0.1 + 0.03V - 0.0005V^2$.
- Equation governing oxide width: $w(t,V) = w_0(V) + w_1(V)\ln(t)$
  $w_0(V) = 11.6 + 9V$ and $w_1(V) = 2.7 + 0.9V$.

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[a] M. Calleja and R. García, "Nano-Oxidation of Silicon Surfaces by Noncontact Atomic-Force Microscopy: Size dependence on Voltage and Pulse Duration," *Applied Physics Letters*, vol.76, no.23, pp.3427-3429, 2000.

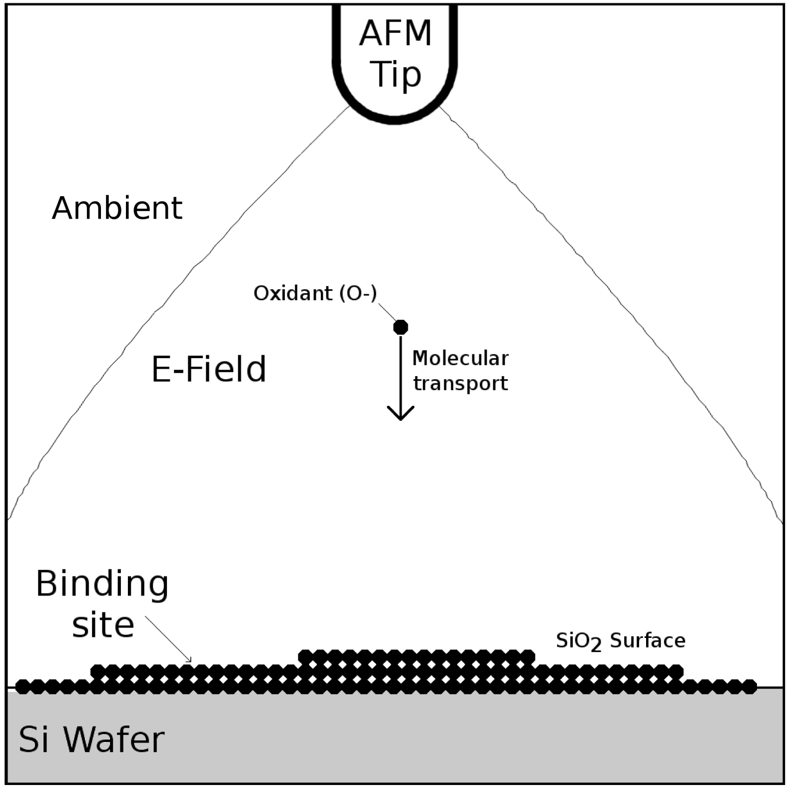
AFM Nanodot

- Equation for nanodot height and width, including pulse time, voltage, and humidity:

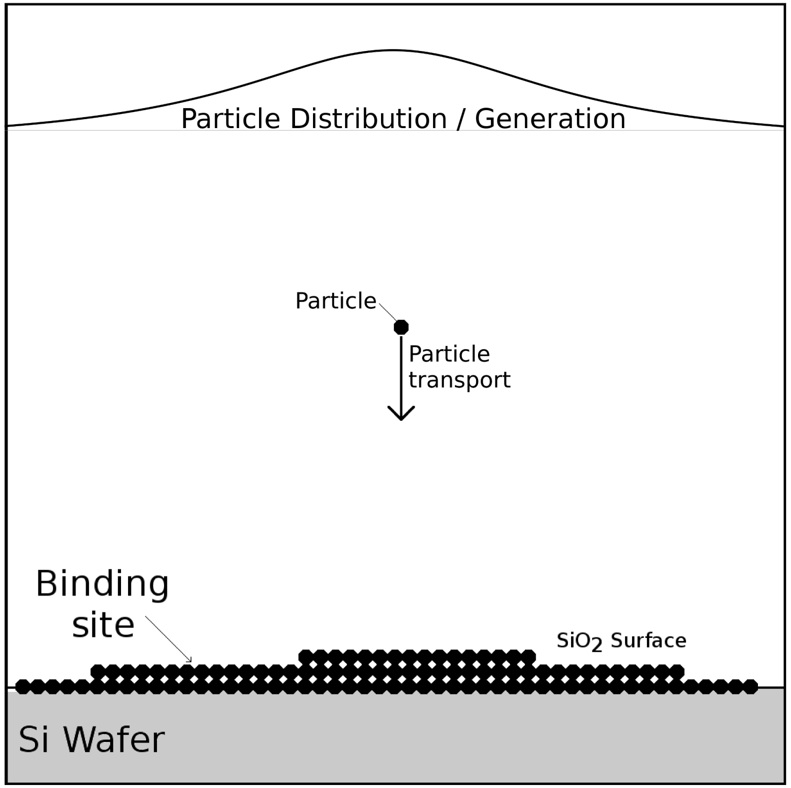
$$H(t,V,h) = \left[\left(-2.1 + 0.5V - 0.006V^2\right) + \left(0.1 + 0.03V - 0.0005V^2\right) ln\left(t\right)\right] \times \left[0.00037h^2 - 0.019h + 0.928\right],$$

$$W(t,V,h) = \left[(11.6 + 9V) + (2.7 + 0.9V)\, ln(t)\right] \times \left[0.019h - 0.051\right].$$

Introduction - AFM Oxidation Kinetics



() Oxidation kinetics



() Oxidation kinetics model

Modeling AFM Oxidation

- Generate particle at position $p_0(x_0,y_0,z_0)$.

x_0 and y_0 are Lorentzian-distributed random variables,
z_0=d is the effective vertical position of the static dot charge.

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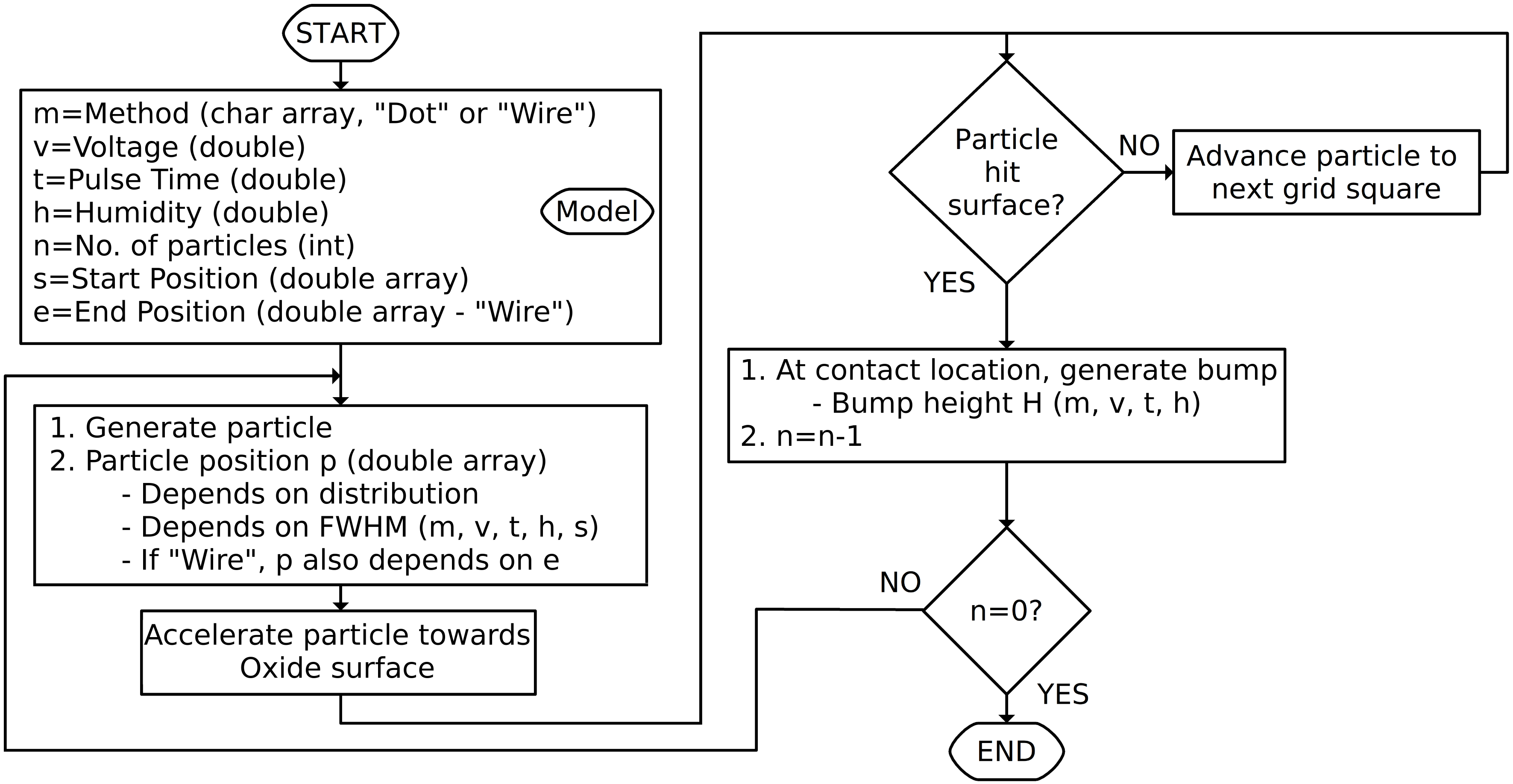
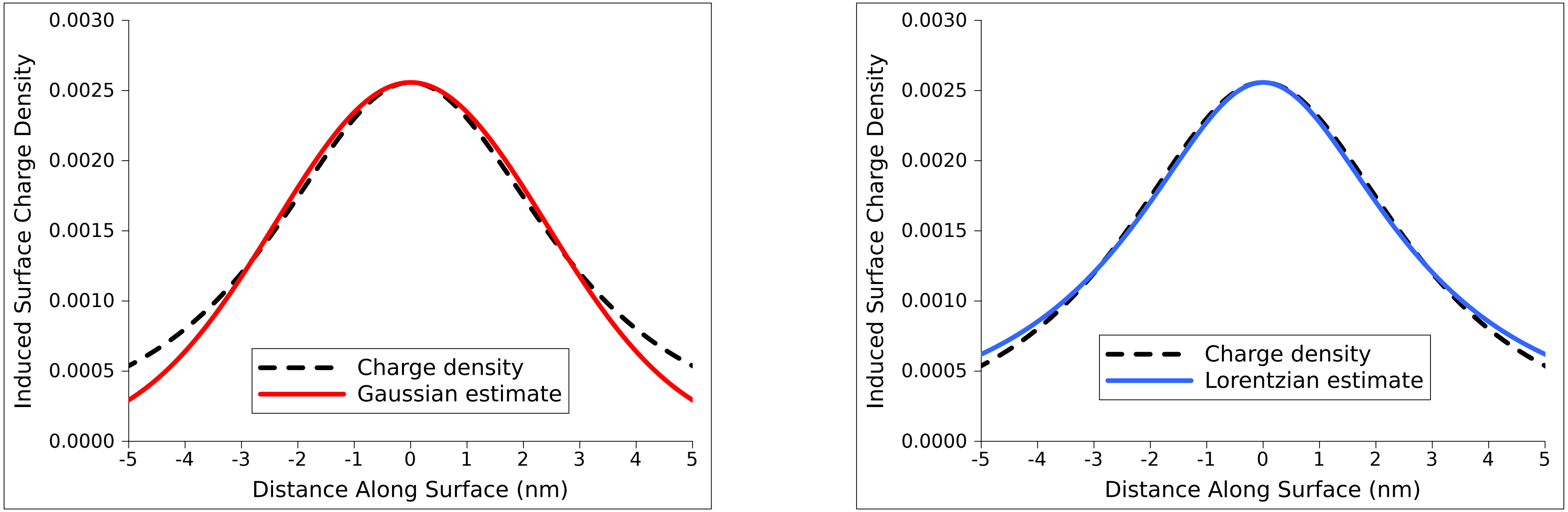
- If the number of particles is 0 the simulation is complete.

Otherwise the variable used to keep track of the remaining particles must be reduced by 1 and the procedure must be repeated from Step 1.

AFM Oxidation Simulator



Gaussian and Lorentzian Distributions



Comparison of Gaussian and Lorentzian distributions with the induced surface charge density model.

Algorithm for the Gaussian Model

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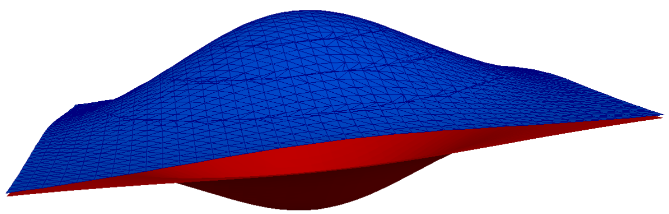
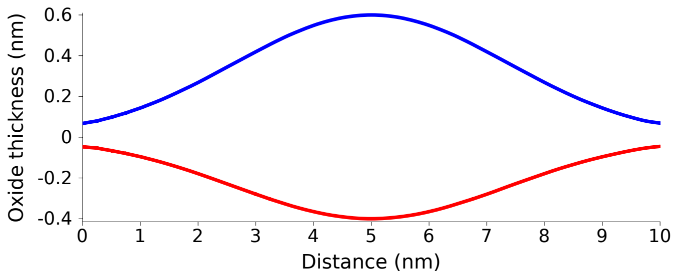
- Must generate evenly distributed circle with unity radius $r^2 = x_0^2 + y_0^2$ with coordinates (x_0,y_0).
- Gaussian distributed coordinates (Marsaglia polar method) are then:

$$x = x_0\sqrt{\frac{-2ln\left(r^2\right)}{r^2}}, y = y_0\sqrt{\frac{-2ln\left(r^2\right)}{r^2}}.$$



(d) Gaussian nanodot and its



(d) diagonal cross section

Lorentzian Distribution

- Probability density function of the Lorentzian distribution:

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- Quantile function of the Lorentzian distribution:

$$r_x = \frac{1}{\Phi\left(p\right)} \equiv \gamma \cdot tan\left[\pi\left(p - \frac{1}{2}\right)\right],$$

2γ is the interquartile range

p is an evenly distributed random number between 0 and 1

Two-Dimensional Lorentzian Distribution - Attempt 1

- Distribute particle evenly around needle tip:

```
do {
    v0=1*RandomNumber();
    v1=1*RandomNumber();
    r_sq=v0*v0+v1*v1;
  } while (r_sq>=1);
  r=sqrt(r_sq);
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- Generate evenly distributed angle θ between 0 and 2π.

- Final particle position is given by $(x_0, y_0) = (r_x \cos\theta, r_x \sin\theta)$.

Two-Dimensional Lorentzian Distribution - Attempt 2

- Form an area integral for polar coordinates:

$$\int_0^{\infty}\int_0^{\infty}\varphi\left(x,y\right)dxdy=\int_0^{2\pi}\int_0^{\infty}\eta\left(r,\theta\right)rdrd\theta.$$

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- The One-dimensional probability distribution must then be integrated:

$$\xi_r = \int_0^{r_x} \frac{1}{\pi} \cdot \frac{1}{1+r^2} \cdot r \cdot dr$$

ξ_r is an evenly distributed value and r$_x$ is a value distributed with the Lorentzian distribution.

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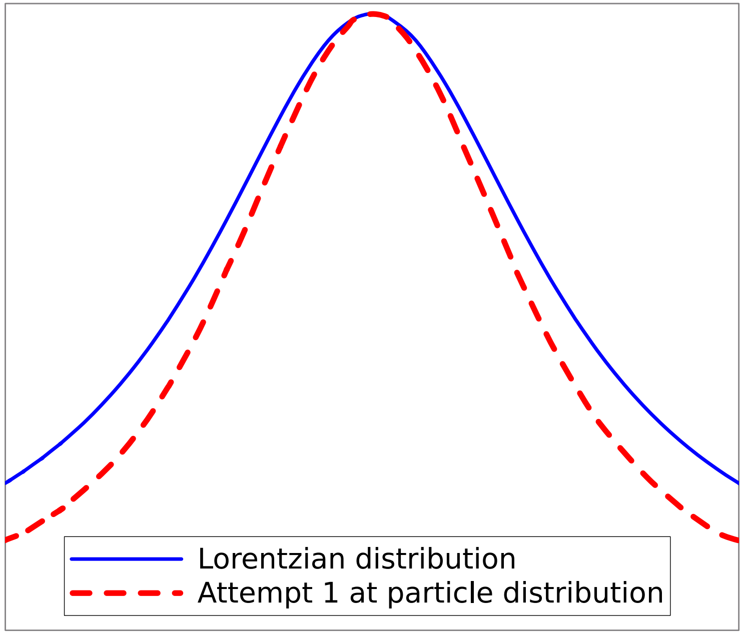
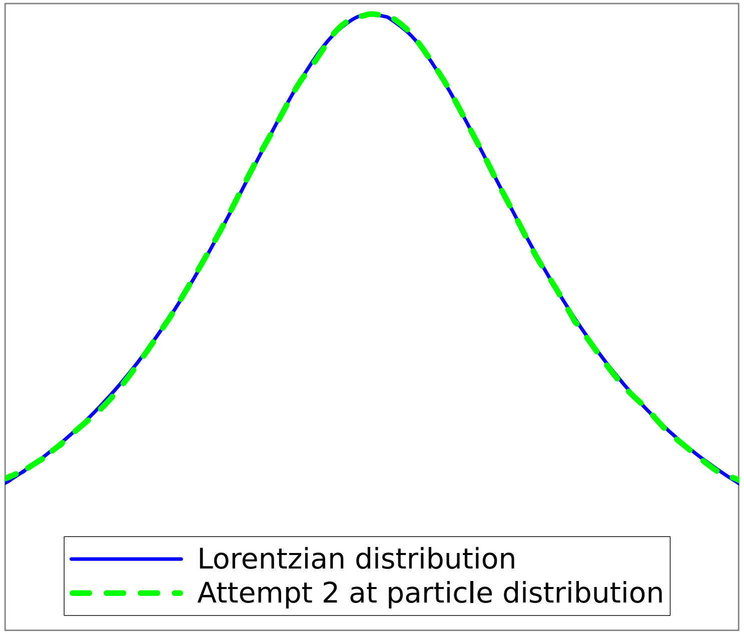
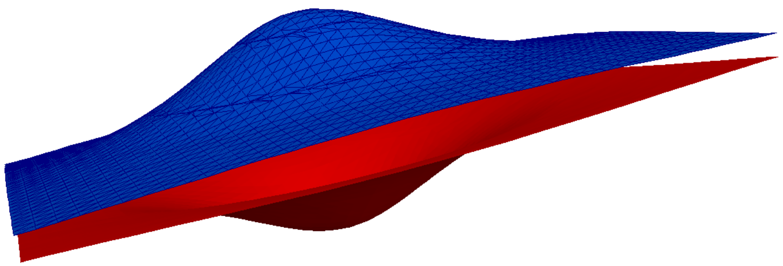
- Angle θ between 0 and 2π is generated and final particle position is given by $(x_0,y_0) = (r_x\cos\theta, r_x\sin\theta)$.

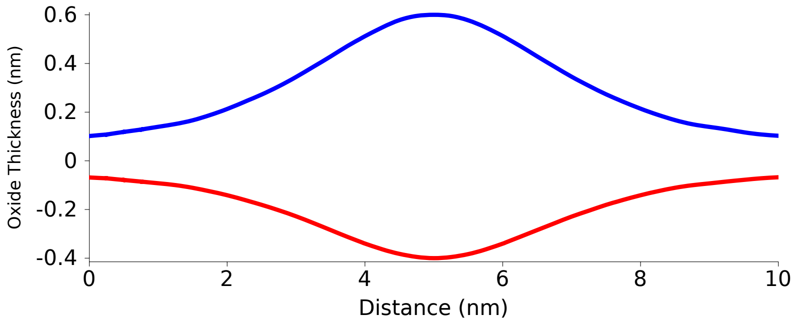
Gaussian Model Example





Lorentzian nanodot example:





Conclusion

- AFM is used as a lithographic technique capable of manufacturing nanometer-sized devices.
- Two-dimensional Lorentzian distribution is developed for an AFM simulator.
- Monte Carlo method is implemented to generate particles around the needle tip.
- Particles are accelerated and collide with the Level Set surface.
- Generated nanodot follows a Lorentzian probability distribution.