Chapter 11

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

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Abstract. Atomic force microscopy (AFM) is a lithographic technique capable of manufacturing nanometer-sized devices. A Monte Carlo simulator for oxide growth on a silicon substrate using the AFM method is described. In previous publications, it is shown that a nanodot formed using AFM has a diagonal cross section that closely resembles the Lorentzian distribution. Therefore, an essential part of the simulator is the generation of particles using a two-dimensional Lorentzian distribution around the AFM needle tip. A successful algorithm was generated by integrating the probability distribution, while taking into consideration two-dimensional pieces of the surface. A second evenly-distributed value is used to generate a radial distribution θ. The location of each generated particle is then described by $(x,y) = (r_x \cos \theta, r_x \sin \theta)$.

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Mathematics Subject Classification 2010. 00A72, 65C05, 65C10, 65C17.

11.1   Introduction

Atomic force microscopy (AFM) [1] was developed in 1986 as a method to detect depressions and protuberances on a nanometer-sized section of a sample surface. Following this initial discovery, the use of an atomic force microscope was also shown to be an effective tool in the oxidation of nanometer-sized patterns on a silicon wafer [2]. Furthermore, it has been extensively used not only in the semiconductor industry, but also in physics, chemistry, biology, biochemistry, and other disciplines where the chemical or physical properties of a surface are required [3]. The AFM lithographic technique is capable of manufacturing nanometer-sized devices and is a promising alternative to modern lithographic methods. Performing physical simulations to replicate the AFM process is currently not feasible for large surface simulations, and therefore a Monte Carlo approach must be considered. Previous research has shown that a simulator for the generation of AFM nanodots is feasible in a Level Set environment [4] using empirical equations for the nanodot height and full width at half maximum (FWHM). It has also been shown that the physical shape of an oxide dot, generated using AFM, most closely resembles a Lorentzian distribution when viewed in

diagonal cross sections [5]. Therefore, it is the goal of this work to create a Monte Carlo simulator for an AFM nanodot following a two-dimensional Lorentzian distribution around the AFM needle tip.

The simulator must be seamlessly integrated into an existing Level Set simulator environment, which is described in detail in [6]. The wafer surface and surfaces where differing materials intercept, such as the silicon–silicon-dioxide interface, are described using the Level Set equation. The equation describing the effect of the processing conditions, including bias voltage, process time, and ambient humidity, on the height and FWHM of the oxide nanodot is

$$H(t, V, h) = [H_1(V) + H_2(V) \, ln(t)] \left[0.00037h^2 - 0.019h + 0.928\right],$$
$$W(t, V, h) = [(11.6 + 9V) + (2.7 + 0.9V) \ln(t)] [0.019h - 0.051],$$

where $H_1 = -2.1 + 0.5V - 0.006V^2$ and $H_2 = 0.1 + 0.03V - 0.0005V^2$.

11.2   Modeling Oxidation Kinetics

Figure 11.1a shows a simplified version of the kinetics of AFM oxidation. A charged AFM tip is brought near a grounded silicon surface, resulting in the generation of an electric field. This field breaks up the ambient into ions and causes the downward acceleration of oxyions (O^-, OH^-) towards the surface. The combination of these ions with the silicon surface results in the generation of SiO_2. The model implemented to mimic oxidation kinetics is similar to the method described in [5]. Particles are generated around the needle tip with a desired two-dimensional distribution. Each particle is
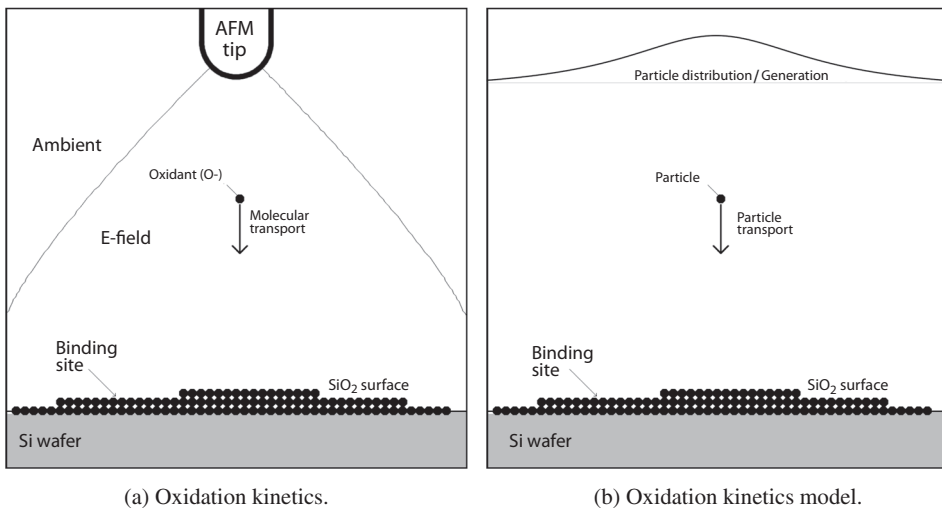

(a) Oxidation kinetics.   (b) Oxidation kinetics model.

Figure 11.1. The AFM tip is modeled by generating particles generated around the needle tip, following a desired distribution.

accelerated towards the silicon surface, causing a "bump" upon impact. The summation of all particles generates the desired nanodot shape on the surface. In [5] particles are generated using an even distribution. The Monte Carlo rejection technique is then implemented to select the particles to be used for the nanostructure. The Monte Carlo rejection techniques is not feasible when nanosized structures are required to be simulated on millimeter sized wafers.

Therefore, a more direct Monte Carlo approach must be taken to simulate nanodots and nanowires. The implementation of the simulator is as follows:

1. Generate a particle at position $p_0(x_0, y_0, z_0)$, located on a plane parallel to the silicon surface with a desired distribution (Gaussian or Lorentzian), as shown in Figure 11.1b. x_0 and y_0 are distributed random variables, while $z_0 = d$ is the effective vertical position of the static dot charge.

2. Accelerate the particle towards the silicon surface along the vertical direction, until it collides with the top surface.

3. At the impact location, advance the ambient–oxide interface towards the ambient while advancing the oxide–silicon interface into the silicon.

4. If the number of particles is 0 the simulation is complete. Otherwise particle counter must be reduced by 1 and the procedure must be repeated from Step 1.

The processing steps required to simulate AFM using a Monte Carlo method with a Gaussian or Lorentzian distribution of particles is shown in Figure 11.2.
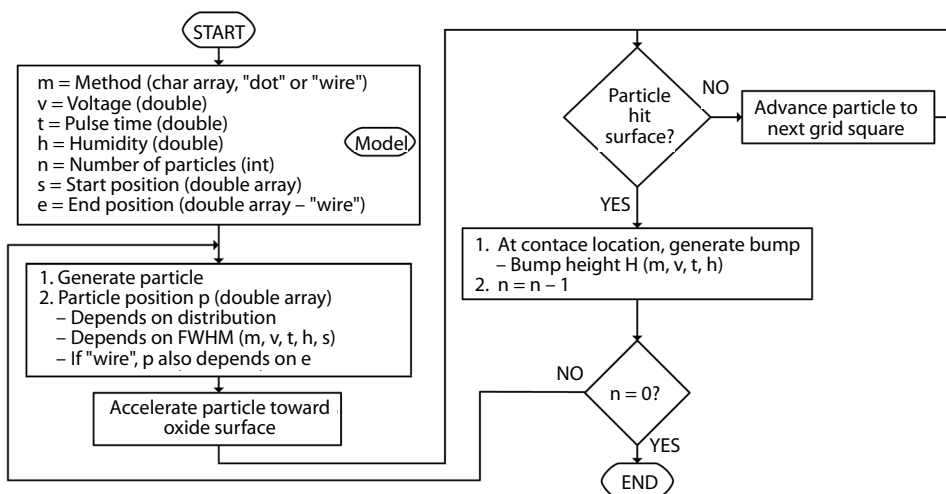

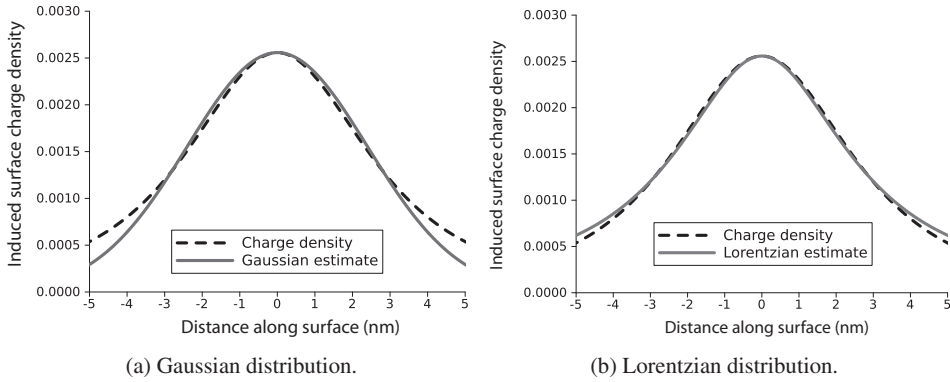**Figure 11.2.** Flow chart for the Monte Carlo AFM simulator in a Level Set environment.

(a) Gaussian distribution.   (b) Lorentzian distribution.

Figure 11.3. Difference between Gaussian and Lorentzian distributions.

11.3   Development of the Lorentzian Model

As seen from the previous discussion regarding the Monte Carlo model for AFM oxidation from Figure 11.2, a method to distribute particles according to a desired distribution is required. The Gaussian distribution is well known; however, in a previous publication [5] it was found that a Lorentzian distribution is a better fit to the final shape of a desired nanostructure, as can be seen in Figure 11.3.

The implementation of the Gaussian distribution was performed successfully, while a similar approach to the Lorentzian distribution was attempted without much success. Therefore, in order to generate particles according to a Lorentzian distribution, a novel approach was developed.

11.3.1   Algorithm for the Gaussian Model

The quantile function of the one-dimensional Gaussian distribution, required for the generation of a random particle position x_r, is

$$x_r \equiv \sqrt{2}\, \mathrm{erf}^{-1}\left(2u - 1\right) \qquad u \in (0, 1)\,. \tag{11.1}$$

Because of the error function, the quantile Gaussian function is not easily implementable in a Monte Carlo environment, and hence another model is desired. The model implemented is based on the well-known Marsaglia polar method [7]. This method suggests a way to generate two independent standard normal random variables. The first step is the generation of an evenly distributed random point (r_x, r_y) within a circle of unity radius $s = r_x^2 + r_y^2$, where r_x and r_y are evenly distributed random numbers $\in (-1, 1)$. The Gaussian distributed coordinates (x,y) can then be

(a) Gaussian nanodot and its
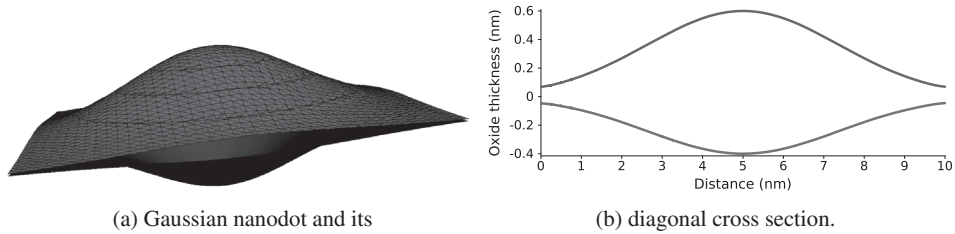
(b) diagonal cross section.

Figure 11.4. Nanodot generated using Gaussian particle distribution.

calculated using the Marsaglia equations:

$$x = r_x \sqrt{\frac{-2\ln(s)}{s}}, \qquad y = r_y \sqrt{\frac{-2\ln(s)}{s}}. \tag{11.2}$$

A sample Gaussian distributed nanodot is shown in Figure 11.4.

11.3.2 Development of the Lorentzian Model

11.3.2.1 One-Dimensional Lorentzian Distribution

The normalized pdf (probability density function) of the Lorentzian distribution is given by

$$f(x) = \frac{1}{\pi} \cdot \frac{1}{1 + x^2}. \tag{11.3}$$

The cpd (cumulative probability distribution) is found by integrating the probability density function $\Phi(x) = \int_{-\infty}^{x} f(u)\,du$

$$\Phi(x) = \frac{1}{\pi} \arctan(x) + \frac{1}{2}. \tag{11.4}$$

The quantile function of the Lorentzian distribution, required for particle generation, is the inverse cpd

$$x_r = \Phi^{-1}(u) \equiv \tan\left[\pi\left(u - \frac{1}{2}\right)\right], \tag{11.5}$$

where $u \in (0, 1)$ is a uniformly distributed random number.

11.3.2.2 Two-Dimensional Lorentzian Distribution

We must perform the same analysis shown for the one-dimensional Lorentzian distribution in order to generate a two-dimensional Lorentzian quantile function. The pdf of the two-dimensional Lorentzian distribution can be represented as

$$f(x, y) = \frac{C}{1 + x^2 + y^2}, \tag{11.6}$$

where C is the normalization constant. Using polar coordinates, where $x^2 + y^2 = r^2$ and $dx\, dy = r\, dr\, d\theta$, it can easily be shown that the pdf cannot be normalized in the whole $\Re^2$. We therefore must normalize the equation to a desired maximum radius $r_{\max}$:

$$1 = 2\pi\, C \int_0^{r_{\max}} \frac{1}{1+r^2} r\, dr = C\, \pi\, \ln\left(1 + r_{\max}^2\right). \tag{11.7}$$

The normalization constant follows from the cpd, normalized to $r_{\max}$:

$$\Phi\left(r\right) = \frac{\ln\left(1 + r_L^2\right)}{\ln\left(1 + r_{\max}^2\right)}, \tag{11.8}$$

where we can treat $\ln\left(1 + r_{\max}^2\right)$ as a $r_{\max}$-dependent constant M. By inverting the cpd and solving for r_L we can find the two-dimensional Lorentzian quantile function, required for particle generation,

$$r_L = \sqrt{e^{u\, M} - 1}, \tag{11.9}$$

where $u \in (0,1)$ is a uniformly distributed random number.

An evenly-distributed angle θ between 0 and 2π is generated, and the final particle position is given by $(x,y) = (r_x \cos\theta, r_x \sin\theta)$. It can be observed that the choice of $r_{\max}$ affects the height of the Lorentzian distribution, thereby affecting the height of the desired nanodot. Therefore, an additional contribution, dependent on $r_{\max}$ is needed in the equation for the height generated by each particle. This contribution is $\ln(1 + r_{\max}^2)$. The resulting nanodot cross section, shown in Figure 11.5 matches the ideal one-dimensional Lorentzian distribution. This method allows for the generation of nanodots, such as the one shown in Figure 11.6, which follow a Lorentzian distribution, as required for the AFM simulator.
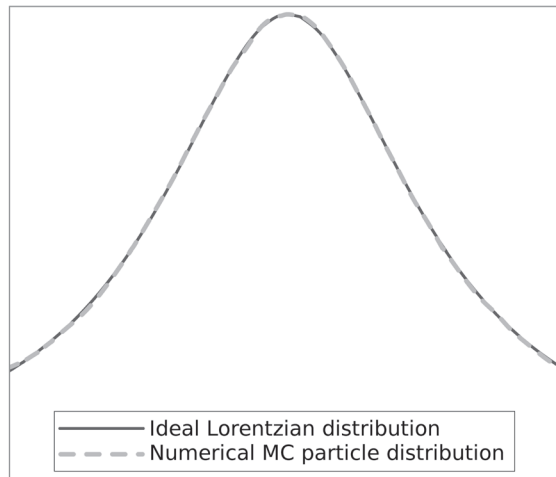

Figure 11.5. Nanodot cross section generated using a Lorentzian distribution.
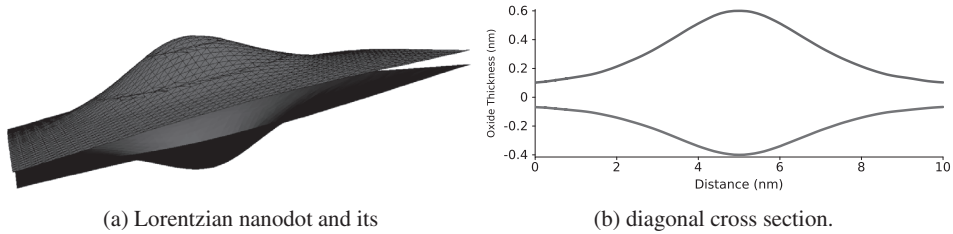
(a) Lorentzian nanodot and its   (b) diagonal cross section.

Figure 11.6. Nanodot generated using Lorentzian particle distribution.

11.3.2.3   Marsaglia Polar Method

The expression for the quantile function in (11.9) suggests a potential connection to the Marsaglia polar method. A Lorentzian distribution can be generated using a similar procedure. The first step is, once again, the generation of a random point (r_x, r_y) within a unit circle with radius $s = r_x^2 + r_y^2$. The Lorentzian distributed coordinates (x,y) can then be expressed as

$$x = r_x \sqrt{\frac{e^{sM} - 1}{s}}, \qquad y = r_y \sqrt{\frac{e^{sM} - 1}{s}}, \qquad (11.10)$$

where $M = \ln\left(1 + r_{max}^2\right)$.

11.4   Conclusion

A two-dimensional Lorentzian distribution of particles is developed for an AFM simulator. The simulator implements a Monte Carlo method to generate particles around the needle tip, which are subsequently accelerated towards the wafer surface, described using the Level Set equation. Once the particles have been generated and accelerated towards the surface, the resulting structure forms an AFM nanodot, the cross section of which follows a Lorentzian probability distribution. A method, similar to the Marsaglia polar method for Gaussian particle generation is implemented to generate Lorentzian distributed particles in two-dimensional space.

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