A Monte Carlo Simulator for Non-contact Mode Atomic Force Microscopy

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Abstract. Nanolithography using Non-Contact Mode Atomic Force Microscopy (NCM-AFM) is a promising method for the manufacture of nanometer sized devices. Compact models which suggest nanopatterned oxide dots with Gaussian or Lorentzian profiles are implemented in a Monte Carlo simulator in a level set environment. An alternative to compact models is explored with a physics based Monte Carlo model, where the AFM tip is treated as a point charge and the silicon wafer as an infinite conducting plane. The strength of the generated electric field creates oxyions which accelerate towards the silicon surface and cause oxide growth and surface deformations. A physics based model is presented, generating an oxide dot based on the induced surface charge density. Comparisons to empirical models suggest that a Lorentzian profile is better suited to describe surface deformations when compared to the Gaussian profile.

1 Introduction

Atomic Force Microscopy (AFM) [1] was developed in 1986 to measure protuberances and depressions on a nanometer sized section of a desired surface. For this purpose AFM has been a useful tool in physics, chemistry, biology, biochemistry, as well as in the semiconductor industry. This method utilizes the Van der Waals interaction between the tip and a sample surface to determine the surface properties [11]. Several years after the development of AFM, it was noted that this method can also be implemented to pattern semiconductor or metal surfaces with nanometer scale precision for processes such as local anodic oxidation of silicon [4]. With the ability to pattern nanoscale devices, the importance of AFM in the semiconductor industry increased significantly. There are various modes in which AFM can operate. The most commonly used for local anodic oxidation of semiconductor surfaces are contact mode (CM-AFM) and non-contact mode (NCM-AFM) [2–4]. NCM-AFM allows narrow patterns to be generated at relatively high speed, making it the preferred method for local anodic nanooxidation of silicon surfaces [7].

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Over the past decades the use of NCM-AFM as a tool for the local anodic oxidation of semiconductor surfaces has significantly increased, generating a demand for a simulation tool which predicts semiconductor surface deformation due to AFM processing. Conventional photolithographic methods are unable to accurately describe the processing steps necessary to generate a nanoscale device using AFM. Having the ability to simulate the AFM process is essential in order to understand the extent of devices which can be manufactured using this method. In this work, we present an analytical model implemented using a Monte Carlo simulator in a level set environment [6]. The level set simulator is an existing silicon process simulator which describes surface deformations after conventional processing steps are performed on a silicon surface [5]. The final deformation of a silicon surface after local anodic nanooxidation using NCM-AFM can either have a Gaussian [10] or a Lorentzian [8] profile.

We further explore an alternative to this compact model by developing a physics based Monte Carlo model, where the AFM needle tip is treated as a point charge which generates an electric field towards the silicon surface. The silicon surface is treated as an infinite conductive plane, since the silicon wafer extends to lengths much longer than the nanoscale AFM tip distance. With this physics based Monte Carlo model, the validity of the available analytical model is explored and the final shape of a silicon wafer dot after applying AFM nanolithographic processing steps is generated. Using the results, a suggestion will be made whether to use a Gaussian or Lorentzian profile for the analytical model. The processing steps for a physics based Monte Carlo approach are introduced.

2 Non-Contact Mode Atomic Force Microscopy

AFM is a relatively modern lithographic technique, capable of generating patterns on semiconductor surfaces through the application of an electric field. It is a very useful tool for local anodic nanooxidation of silicon surfaces. Fig. 1 shows the schematic of NCM-AFM, where the tip is placed near the silicon surface and a negative bias voltage, relative to the silicon potential, is applied. An electric field is generated between the AFM tip and the silicon wafer. The high electric field near the AFM tip causes the creation of oxyions (O^- and OH^-) from the air ambient, which are then accelerated towards the silicon surface, away from the negatively charged AFM tip. The oxyions react with the silicon substrate, resulting in the generation of silicon dioxide which is simultaneously expanded into the silicon substrate and the ambient. A detailed explanation of the AFM method and its use to physically or chemically modify surfaces at nanometer scales can be found in [11].

3 Empirical Atomic Force Microscopy Model

An empirical model for the generation of an oxide dot using local anodic nanooxidation of silicon surfaces with the NCM-AFM method was presented in [2].

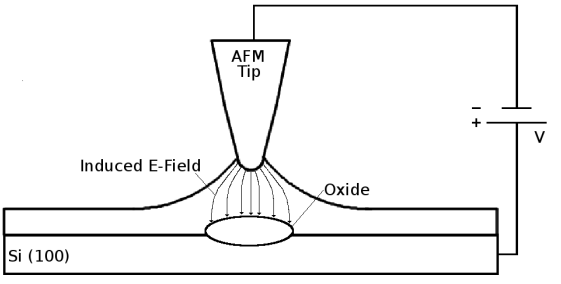

Fig. 1. Basic schematic for the local anodic nano-oxidation of silicon surfaces using NCM-AFM

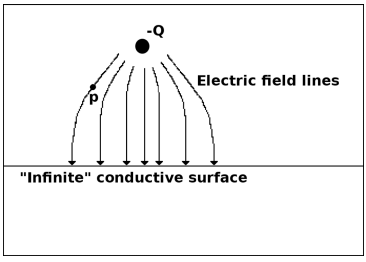

Fig. 2. AFM tip is treated as a point charge in order to create a physics based Monte Carlo simulation model

It is suggested that the width and height of an oxide dot have a linear dependence on the applied bias voltage, while a logarithmic dependence exists for the pulse duration. An empirical equation which governs the height of the oxide dot produced with NCM-AFM mode has been presented in [2]

$$h\left(t,V\right)=h_0\left(V\right)+h_1\left(V\right)\ln\left(t\right), \tag{1}$$

where $h_0\left(V\right)=-2.1+0.5V-0.006V^2$ and $h_1\left(V\right)=0.1+0.03V-0.0005V^2$, and the size, voltage, and time are expressed in nanometers, volts, and seconds, respectively. Similarly, the equation which governs the width of the oxide dot, represented as the full width at half maximum (FWHM) is

$$w\left(t,V\right)=w_0\left(V\right)+w_1\left(V\right)\ln\left(t\right), \tag{2}$$

where $w_0\left(V\right)=11.6+9V$ and $w_1\left(V\right)=2.7+0.9V$, and the size, voltage, and time are expressed in nanometers, volts, and seconds, respectively.

3.1 Monte Carlo Simulation Approach

An analytical simulator for NCM-AFM was created in the level set environment described in [6] with a Monte Carlo method as shown in Fig. 3. The Monte Carlo technique is performed by generating a desired number of particles, distributed using a selected probability distribution along a plane parallel to the silicon surface, ensuring that the FWHM fits with (2). Each particle is accelerated towards the silicon surface. After a collision with the surface, the silicon dioxide is expanded by a height determined by (1) and the total number of particles. After all the particles have been simulated, the result is a surface topography of a nanodot with a height and width dependent on (1) and (2), respectively. An example from [2] is simulated at a bias voltage of 20V and a pulse time of 0.125ms, resulting in a height and width of 1nm and 5.6nm, respectively, shown in Fig. 4.

The results of the experiments from [2] and the analytical model were used in order to construct a physics based model for NCM-AFM in Section 4.

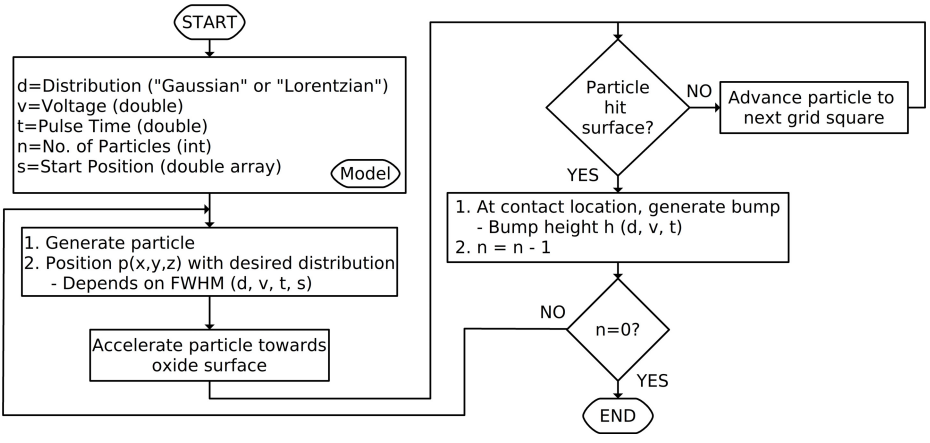

Fig. 3. Flow chart for the analytical Monte Carlo NCM-AFM simulator

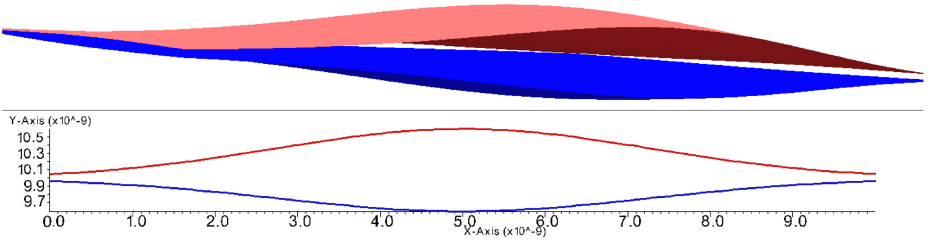

Fig. 4. AFM simulation: bias voltage is 20V and pulse width is 0.125ms. Top surface is the oxide-ambient interface, while the bottom surface is the oxide-silicon interface.

3.2 Lorentzian versus Gaussian Profiles

There are a very limited number of simulators which can deal with NCM-AFM nanooxidation, therefore there is not a clear consensus on the exact structure of the final oxide dot. The important feature of the nanodot is its height and FWHM. However, in order to create a simulator for NCM-AFM, more information is required. Some literature states that the final oxide dot approximately follows a Gaussian curvature [10], while some suggest a Lorentzian profile [8]. The differences between the two options are shown in Fig. 5 where the cross-section of a NCM-AFM simulation is depicted. The simulation is performed with the bias voltage set to 20V and a pulse time of 0.125ms. According to the model described in Section 3.1 a height of 1nm and a width of 5.6nm are achieved.

From Fig. 5 it is evident that both curves have the same height and width, since the points of intersect for the two curves are at $\pm\frac{1}{2}FWHM$. The difference is that the Lorentzian profile suggests that the oxide expands laterally near the silicon interface, while the Gaussian profile has a steeper curve, resulting in slightly more oxide in the top half of the nanodot.

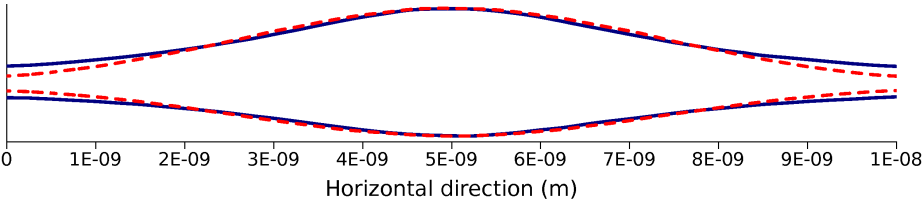

Fig. 5. Cross-section of the oxide pattern when using Gaussian (red-dashed line) distribution and Lorentzian (blue-solid line) distribution

4 Electric Field and Ambient Profiles

In order to simulate the AFM oxidation process with a physical model, the tip of the cantilever from Fig. 1 is treated as a negatively charged stationary dot, while the silicon wafer is treated as an infinitely long conducting plane, shown in Fig. 2. The generated oxyions (particle p from Fig. 2) will move through the ambient towards the silicon surface aided by the electric field. It is assumed that the silicon surface is on the x-y plane, at z=0, the origin p(0,0,0) is located on the silicon surface directly below the charged dot, and the charged dot is at a distance d away from the silicon surface. The equation for the strength of the electric field at a point p(x,y,z) is well known. It is calculated by assuming the presence of an oppositely charged stationary dot located at (0,0,-d) and implementing the image charge method [9]. This method is used in order to calculate the effective charge of the AFM needle tip, the electric field between the AFM tip and the silicon surface, as well as the surface charge density on the silicon surface. The equation which governs the electric potential at a point p(x,y,z) is

$$V\left(\overrightarrow{p}\right) = k\left[\frac{Q}{\left(x^2+y^2+(z-d)^2\right)^{1/2}} - \frac{Q}{\left(x^2+y^2+(z+d)^2\right)^{1/2}}\right], \tag{3}$$

where $k = 1/\left(4\pi\epsilon_0\right)$, Q is the charge at a distance d from the surface. The voltage at p(0,0,d) is known, since this is the applied bias voltage. Using (3), we can find the effective dot charge Q to simulate the AFM tip.

$$\begin{aligned} E_x &= kQ\left[\frac{x}{\left(x^2+y^2+(z-d)^2\right)^{3/2}} - \frac{x}{\left(x^2+y^2+(z+d)^2\right)^{3/2}}\right] \\ E_y &= kQ\left[\frac{y}{\left(x^2+y^2+(z-d)^2\right)^{3/2}} - \frac{y}{\left(x^2+y^2+(z+d)^2\right)^{3/2}}\right] \\ E_z &= kQ\left[\frac{z-d}{\left(x^2+y^2+(z-d)^2\right)^{3/2}} - \frac{z+d}{\left(x^2+y^2+(z+d)^2\right)^{3/2}}\right] \end{aligned} \tag{4}$$

The induced surface charge density is represented as $\sigma\left(x,y,0\right) = \epsilon_0 E_z\left(x,y,0\right)$, leading to the expression

$$\sigma\left(x,y,0\right) = -\frac{d\,Q}{2\pi\left(x^2+y^2+d^2\right)^{3/2}}. \tag{5}$$

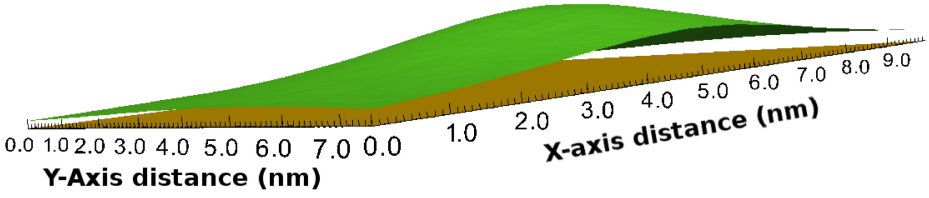

Fig. 6. Shape of the induced surface charge density above the silicon surface

Using the example from [2], modeled with the empirical simulator from Section 3, (3), and (5) we developed a physics based Monte Carlo model for the final pattern of the oxide nanodot.

4.1 Surface Charge Density Modeling

In order to obtain the final pattern for an oxide nanodot generated using NCM-AFM, the physical equations of Section 4 will be implemented for the example from Section 3.1. The initial steps used to generate an oxide nanodot were:

1. Calculate Q based on the applied voltage (20V) and (3) in order to obtain a dot charge of -2.2×10^{-19}C.
2. Using (5) and the known value of the FWHM (5.6nm), calculate the effective location of the dot charge above the silicon surface, d=3.7nm.
3. Using the effective location of the dot charge above the silicon surface, generate an induced surface charge density curve, shown in Fig. 8 and Fig. 9.
4. Use the Monte Carlo rejection technique in order to distribute particles around the AFM tip according to the induced surface charge density, as shown in Fig. 6 and further detailed in Section 5.

5 Monte Carlo Model Implementation

The implementation of the Monte Carlo rejection technique in order to distribute a desired number of particles according to the electric field strength and induced surface charge density is as follows:

1. Generate an evenly distributed particle at position $p_0(x_0,y_0,z_0)$, located on a plane parallel to the silicon surface. x_0 and y_0 are evenly distributed random variables, while z_0=d is the effective vertical position of the static dot charge.
2. Calculate the induced surface charge density $\sigma(x, y, 0)$ at $p_0(x_0,y_0,0)$ using (5).
3. Calculate the maximum induced surface charge density $\sigma_{max}(0, 0, 0)$, at position $p_{max}(0,0,0)$.
4. Generate an evenly distributed random number ρ between 0 and σ_{max}.
5. If $\rho > \sigma(x, y, 0)$ remove the particle and repeat the procedure from step 1. If $\rho \leq \sigma(x, y, 0)$ continue to the next step.

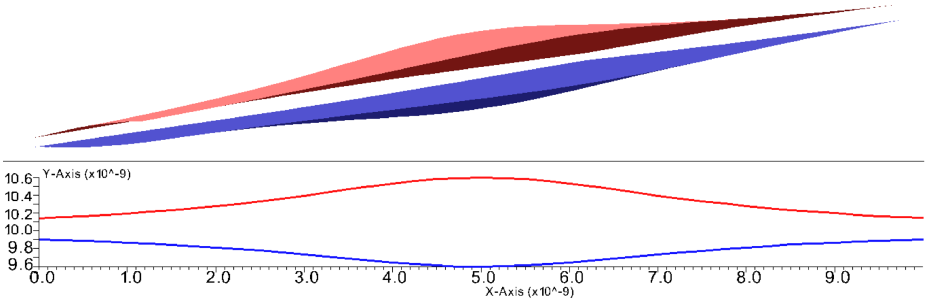

Fig. 7. Surface topography obtained with the presented model

6. Accelerate the particle towards the silicon surface along the vertical direction, until it collides with the surface.
7. At the impact location, advance the ambient-oxide interface towards the ambient while advancing the oxide-silicon interface towards the silicon.
8. If the number of particles is 0 the simulation is complete. Otherwise reduce the number of particles by 1 and repeat the procedure from step 1.

The surface topography, following the above simulation steps, is shown in Fig. 7, where the top and bottom surfaces are the final oxide-ambient and oxide-silicon interfaces, respectively. The induced surface charge density curve is compared to empirical simulations using Gaussian and Lorentzian distributions in Fig. 8 and Fig. 9, respectively. It is immediately evident that the Lorentzian distribution is a better fit to the physics based model. The Gaussian distribution has a sharp slope, which fails to properly show the lateral extension of the oxide nanodot.

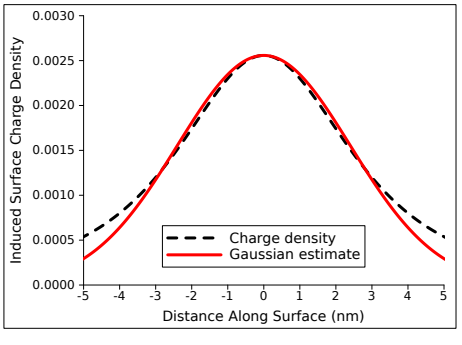

Fig. 8. Comparison to simulation with a Gaussian distribution

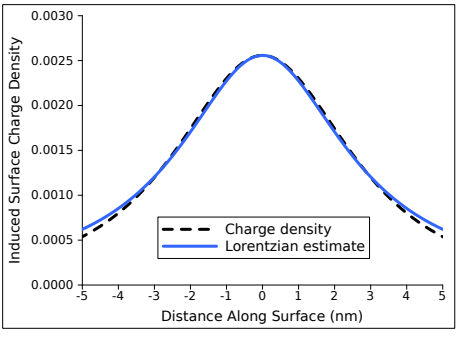

Fig. 9. Comparison to simulation with a Lorentzian distribution

6 Conclusion

Modern lithographic methods are reaching the edge of their potential and nanolithography using NCM-AFM is a promising alternative for the manufacture of nanometer sized devices. A compact Monte Carlo simulator for NCM-AFM is implemented to simulate nanodots based on empirical models. Various publications suggest that surface deformations due to AFM have a Gaussian or Lorentzian profile. A physics based Monte Carlo model, treating the AFM tip as a static charge which generates an electric field towards the silicon surface, was created. Using a Monte Carlo rejection technique, the induced surface charge density is used as the basis of the final topography. The model shows a better fit to the Lorentzian distributed empirical model when compared to the Gaussian model.

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