A Level Set Simulator for Nanooxidation using Non-Contact Atomic Force Microscopy

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***Abstract*—Atomic force microscopy (AFM) can be used as a lithographic technique capable of manufacturing nanometer-sized devices. A simulator for AFM, implemented in a Level Set environment, is presented. The simulator uses empirical models to deduce the shape of a desired nanodot based on the applied voltage, pulse time, and ambient humidity. The shape of an AFM nanowire depends on the same factors as the shape of the nanodot in addition to the wire's orientation with respect to the (010) direction. An advantage of the presented approach is the ease with which further processing steps can be simulated in the same environment. Sample oxide nanodots and nanowires are analyzed, showing the ability of the process to generate nanometer sized structures.**

I. Introduction

Conventional photo-lithographic methods are not able to accurately describe the processing steps required for nano-lithography of modern devices, such as those manufactured with the aid of an atomic force microscope (AFM) [1], shown in Figure 1. AFM was initially developed as a method to detect depressions and protuberances on a nanometer sized section of a sample surface [2] using the tunneling current between a conductive cantilever tip and a grounded sample surface. More

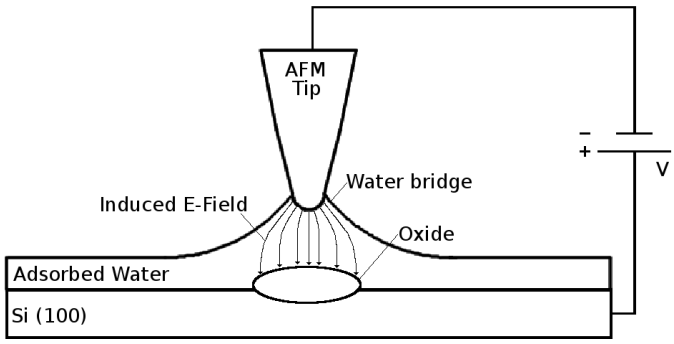

Fig. 1. Basic schematic of AFM oxidation.

recently, AFM has been used as a tool for local anodic oxidation of silicon surfaces, which has been used as a patterning tool for the deposition, removal, and modification of material surfaces with nanoscale precision, mainly for low volume manufacturing (LVM) [3]–[5]. The nanolithography of modern transistors using non-contact mode atomic force microscopy (NCM-AFM) is a promising method for the manufacture of the next generation of nanometer-sized devices [6]–[9]. AFM has been used extensively, 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 [10].

It is becoming critically important to properly model silicon surface deformations due to AFM, since simulating processing steps and the resulting features gives clues to the full potential of device processing with this method. A simulator for nanooxidation using NCM-AFM is presented, which considers the variation of the oxide structure as a function of the applied voltage, oxidation time, and ambient humidity. The presented work is incorporated into an existing Level Set simulator [11]. This allows for the surface to undergo a variety of processing steps before and after NCM-AFM within the same environment.

II. NCM-AFM Models

A. Nanodot Model

The relationship between the pulse time and applied voltage and the oxide nanodot height and width, calculated as the full width at half maximum (FWHM) as described in [12] is shown in Figure 2. This empirical relationship was programmed into the simulator as suggested in [13] and [14]. It can be deduced that a logarithmic relationship exists between the nanodot size and the pulse time, while a mainly linear relationship exists between the nanodot size and the applied voltage. In [6] and [7] the effect of humidity on the nanodot size is presented and the relationship is shown in Figure 3. The derived empirical equation, which describes the effect of all three parameters (time, voltage, and humidity) on the height and width of the oxide dot in nanometers, produced using NCM-AFM mode is shown in (1), where t is the pulse time in seconds, V is the applied voltage in volts, and h is the ambient humidity in percent.

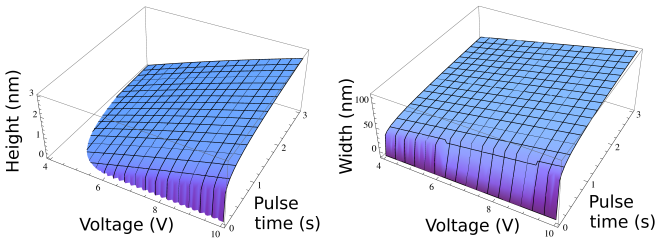

Fig. 2. Voltage and pulse time influence on the oxide dot height and width.

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Nanodot:

$$\begin{aligned} H(t,V,h) &= \left[\left(-2.1+0.5V-0.006V^2\right)+\left(0.1+0.03V-0.0005V^2\right)ln\left(t\right)\right]\times\left[0.00037h^2-0.019h+0.928\right], \\ W(t,V,h) &= \left[\left(11.6+9V\right)+\left(2.7+0.9V\right)ln(t)\right]\times\left[0.019h-0.051\right]. \end{aligned} \tag{1}$$

Nanowire:

$$\begin{aligned} H(t,V,h,\theta) = \;& \left[-0.527-0.45ln\left(0.029-t\right)\right]\times\left(0.56V-2.92\right)\times\left(-0.019h-0.051\right)\times\left(2.2\theta^3-6.02\theta^2+4.1\theta+1\right), \\ W(t,V,h,\theta) = \;& \left[530+107ln\left(t+0.01\right)\right]\times\left(0.0157V^2-0.156V+1.32\right) \\ & \times\left(0.00037h^2-0.019h+0.928\right)\times\left(-0.92\theta^3+1.04\theta^2+1.044\theta+1\right). \end{aligned} \tag{2}$$

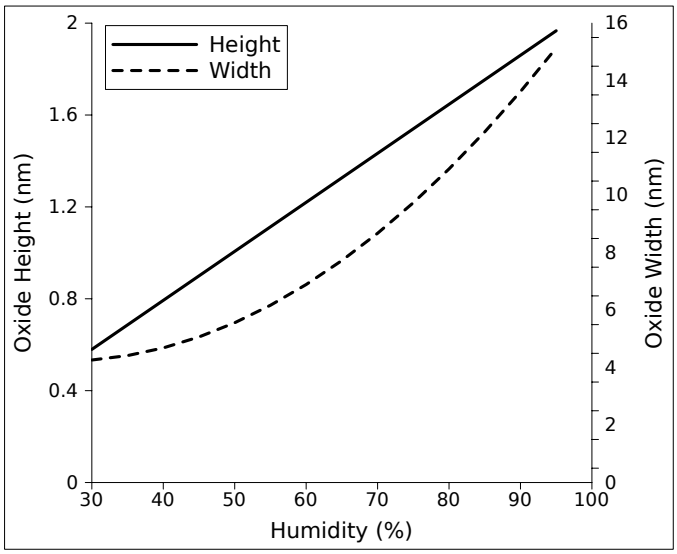

Fig. 3. Effects of humidity on the nanodot height and width.

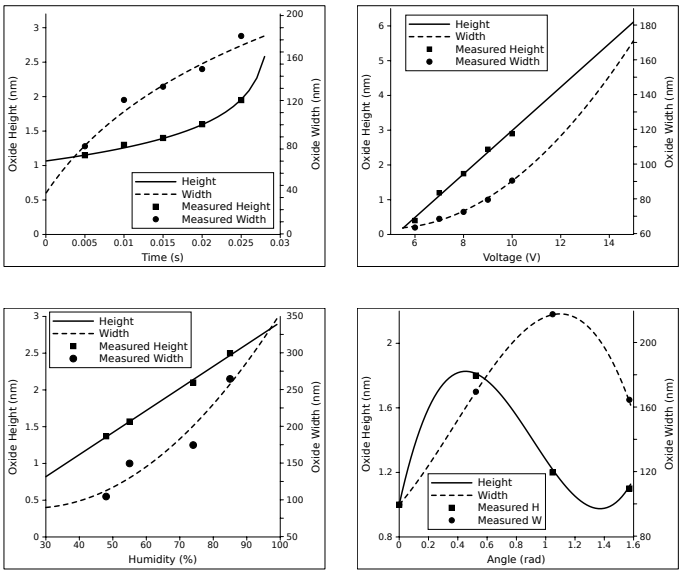

Fig. 4. Effects of time, voltage, humidity, and orientation on the nanowire height and width.

B. Nanowire Model

In addition to the use of experimental observations in order to implement an empirical model for nanodots in the Level Set simulator, the simulator was also extended to include the generation of nanowires using NCM-AFM. From the experimental results found in [7], relevant information was extracted to include the effects on the nanowire shape due to variations in applied voltage, oxidation time, ambient humidity, and wire orientation, shown in Figure 4. The wire orientation is represented as an angle, where the (010) direction is 0^o while (100) is 90^o. It is evident that increasing the oxidation time, the applied voltage, or the ambient humidity results in an increased nanowire height and width. However, the effect of the wire orientation is less predictable. The empirical equation, derived using the experimental results from [7] and implemented in the Level Set simulator is given in (2), where t is the oxidation time in seconds, V is the applied voltage in volts, h is the ambient humidity in percent, and θ is the wire orientation in radians, represented as the angle between the nanowire and the (010) direction.

In Figure 4 the results of our empirical equation (2) are compared to the experimental data from [7].

III. NCM-AFM KINETICS

The procedure implemented to simulate NCM-AFM nanooxidation is similar to the procedure presented in [14]. The Monte Carlo method is used to distribute particles according to a Lorentzian distribution, which are then accelerated towards the silicon surface with ray tracing techniques. The simulator is implemented by first calculating the shape of the nanodot or nanowire with the previously mentioned empirical equations which depend on the oxidation time, applied voltage, ambient humidity, and nanowire orientation. Afterwards, a desired number of particles is distributed above the silicon surface, their position following the pattern of the desired surface deformation. Finally, each particle is accelerated towards the surface, causing it to collide with the wafer. Upon impact, the silicon dioxide is advanced deeper into the silicon, while it simultaneously grows into the ambient. The result is an oxide nanodot or nanowire having the desired height and width, depending on the processing variables of voltage, time, humidity, and orientation. A flow chart which summarizes the simulation steps is given in Figure 5.

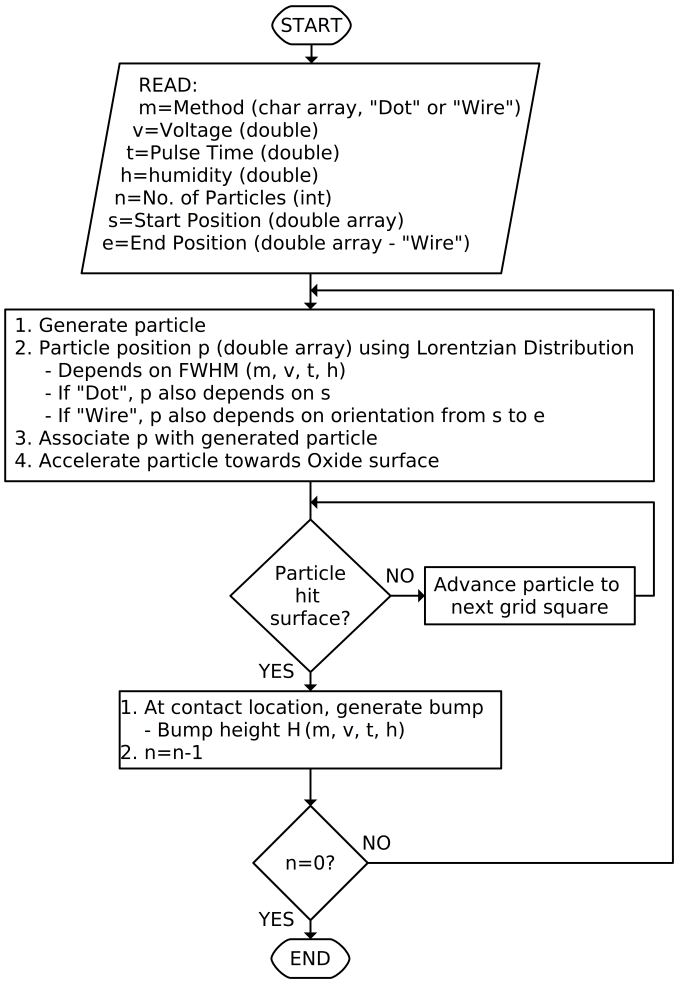

Fig. 5. Flow chart of the simulation process implementing the Monte Carlo method with ray tracing in a Level Set environment.

IV. Sample Simulations

A. Nanodot Simulations

Sample simulations of AFM nanodots are shown in Figure 6. Figure 6(a) shows the distribution of nanodot sizes caused by a variation of pulse times. The voltage and humidity were kept constant at 20V and 55%, respectively, while the time was set to 0.2ms, 0.3ms, 0.5ms, and 1ms. With increasing pulse times, the nanodot height and width also increases, as expected. The height varied from 1.24nm to 2.05nm, while FWHM varied from 15nm to approximately 50nm with pulse time set to 0.2ms and 1ms, respectively.

Figure 6(b) shows the distribution of nanodot sizes caused by a variation of the applied voltage. The pulse time and humidity were kept constant at 0.2ms and 55%, respectively, while the voltage was set to 16V, 18V, 20V, and 22V. With an increasing applied voltage, the nanodot height and width also increases, as expected. The height varied from 0.51nm to 1.58nm, while FWHM varied from 10nm to approximately 18nm with the applied voltage set to 16V and 22V, respectively.

Figure 6(c) shows the distribution of nanodot sizes caused by a variation of the ambient humidity. The pulse time and applied voltage were kept constant at 0.2ms and 20V respectively, while the humidity was set to 30%, 50%, 70%, and 90%. With an increasing ambient humidity, the nanodot height and width also increases, as expected. The height varied from 0.65nm to 2.07nm, while FWHM varied from 10.6nm to approximately 34nm with the ambient humidity set to 30% and 90%, respectively.

The heights shown in Figure 6 are scaled by 20 for improved visualization. The results confirm the experimental results gathered from [6] and [12].

B. Nanowire Simulations

Sample simulations of AFM nanowires are shown in Figure 7. Four wires are generated, each with a different orientation. The wires are generated at 0^o, 30^o, 60^o, and 90^o relative to the (010) direction. The results are summarized in Table 1, where it is evident that the nanowire height and width vary significantly due to a change in the nanowire orientation. All simulations were performed under identical conditions. The oxidation time was set to 0.1ms, the applied voltage was 7V, and the ambient humidity was 55%.

Table 1. Summary of results for the AFM nanowire simulation with varying wire orientation (t=0.1ms, V=7V, h=55%).

Orientation (010)	Height (nm)	FWHM (nm)
0^o	1.07	38.3
30^o	1.93	65.1
60^o	1.30	83.4
90^o	1.19	62.8

The smallest nanowire is noted at an orientation of 0^o, where a height and FWHM of 1.07nm and 38.3nm, respectively, can be observed. The largest nanowire height is noted at 30^o, while the largest FWHM is noted at 60^o. The effect of the wire orientation on the height and width of the nanowire is not identical.

The heights shown in Figure 7 are scaled by 100 for improved visualization. These simulations are confirmed by the experimental observations from [7].

V. Conclusion

AFM is used as a lithographic technique capable of manufacturing nanometer-sized devices. Our simulations of nanodots and nanowires using NCM-AFM in a generic Level Set simulator enable an easy integration with further processing steps. The model for the shape of a desired nanodot or nanowire is generated using empirical equations which describe the effect of various processing conditions on the nanostructure's height and width. The nanodot size is influenced by the pulse time, applied voltage, and humidity, while the nanowire also depends on the orientation. Sample oxide nanodots and nanowires are simulated, showing the ability of the process to generate nanometer sized structures.

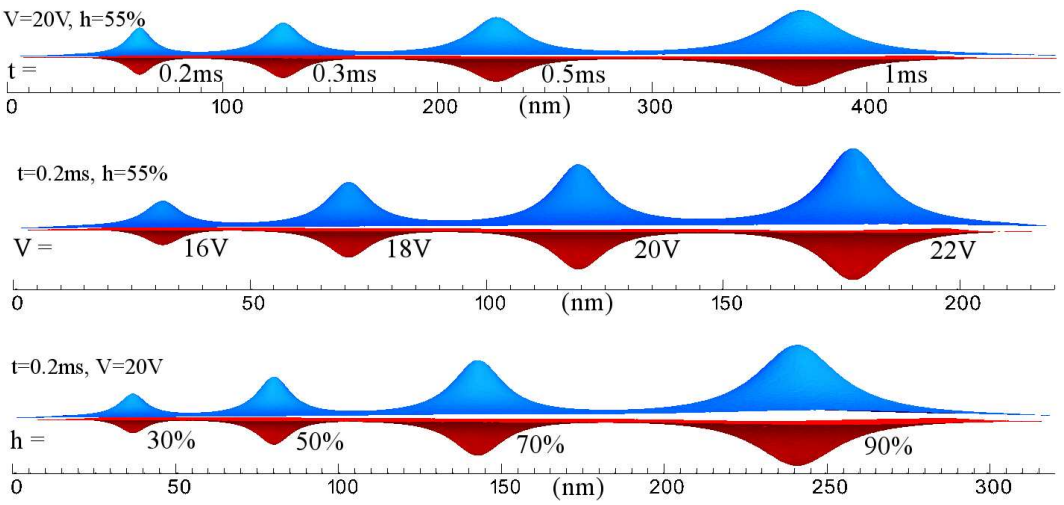

Fig. 6. Effects of time, voltage, and humidity on the nanodot height and width. The vertical axis is scaled by 20 for better visualization. The top surface represents the oxide-ambient interface, while the lower surface represents the oxide-silicon interface.

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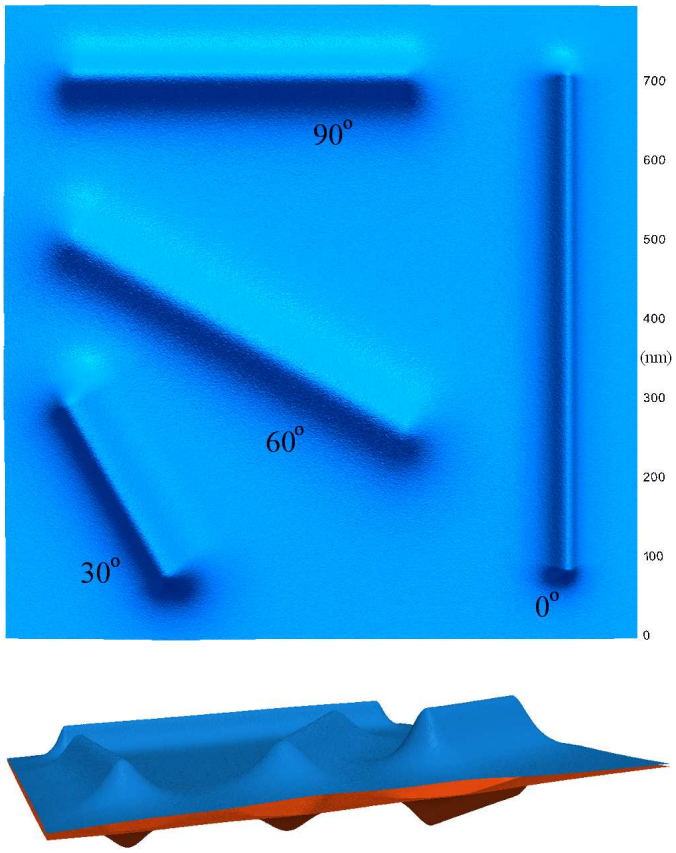

Fig. 7. Effects of wire orientation on the nanowire height and width, with t=0.1ms, v=7V, and h=55%. The vertical axis is scaled by 100 for better visualization. The top surface represents the oxide-ambient interface, while the lower surface represents the oxide-silicon interface.