A SIMULATOR FOR LOCAL ANODIC OXIDATION OF SILICON SURFACES

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ABSTRACT

Models for the local anodic oxidation of silicon using scanning tunneling microscopy and non-contact atomic force microscopy are implemented in a generic process simulator, using the Level Set method. The advantage of the presented implementation is the ease with which further processing steps can be simulated in the same environment. An empirical model for the width of the oxide when using scanning tunneling microscopy is also presented and implemented with the simulator. An oxide dot is simulated for both processes, with a height of 1nm and widths of 5.6nm and 85nm, respectively. The simulator allows for a Gaussian or Lorentzian profile for the final surface deformation.

Index Terms— Atomic force microscopy; Nanolithography; Nanopatterning; Computer aided analysis

1. INTRODUCTION

Scanning tunnel microscopy (STM) [1] was developed in 1982, followed by atomic force microscopy (AFM) [2] in 1986, as methods to utilize tunneling current between a conductive cantilever tip and a sample surface in order to detect depressions and protuberances on a nanometer sized section of the surface. 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 [3].

The local anodic oxidation of semiconductor surfaces was suggested by Dagata et al. [4] as a way to modify semiconductor surfaces with nanometer-scale precision. In this pioneering work, a STM microscope was used to generate features with 100nm resolution by applying a positive bias voltage to the STM needle tip, while keeping the semiconductor surface grounded. Over the years, a negative bias voltage applied to the STM tip proved to produce thicker insulating oxides [5]. The generated electric field, in an oxygen ambient, suggested a potential use of the technology for field-enhanced oxidation at the tip-substrate interface. More recently, the method of local anodic oxidation has been studied and improved to be used as a patterning tool for deposition, removal, and modification of material surfaces with nanoscale precision [6–8]. The generated oxide can act as a mask for subsequent etching steps or as an insulating barrier for thin semiconductor film on insulator processes [9]. Local oxidation nanolithography of graphene using AFM has also shown promise in growing oxide layers [10]. Graphene has recently been demonstrated to provide remarkable electronic properties and large effort is placed towards implementing graphene-based fast electronic and optoelectronic devices [11].

After the initial work with a STM, similar processes have been reported with an AFM microscope with a conductive probe in contact and non-contact modes. A distinct advantage of AFM over STM is its ability to read back the actual topography of the generated pattern, while STM is unable to give the real height [12]. Over the years, empirical and analytical models have been suggested in order to predict how the semiconductor topography changes, when different voltages, pulse times, and tip velocities are applied to the AFM system [4,5,12–18]. This article investigates existing models for the local nano-oxidation of silicon using STM and AFM in order to implement a simulator using a Level Set description of the wafer surface and the expanding oxide.

2. MODELING OXIDATION KINETICS

Local anodic nano-oxidation of silicon surfaces can be performed using STM or AFM in contact mode (CM-AFM) or in non-contact mode (NCM-AFM). It has already been established that AFM in non-contact mode is the preferred method for nanolithography as it is the best compromise between the low 10nm spacial resolution of STM mode with the high speed CM-AFM mode, which can provide thick oxides of up to 8nm. NCM-AFM allows narrow patterns at relatively high speeds [9]. The presented work demonstrates a simulator for STM and NCM-AFM nano-oxidation of silicon wafer surfaces, which is incorporated into an existing topography simulator from [19].

2.1. Simulator Implementation

The simulator presented for the anodic nano-oxidation of silicon is implemented in order to fully function alongside the process simulator presented in [19]. The Level Set method is

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utilized in order to describe the top surface of the wafer and surfaces which separate different materials. It can be used to simulate various photolithographic steps such as etching, deposition, smoothing, and mask application. In order to incorporate oxidation, multiple surfaces must be able to evolve simultaneously at varying velocities, since the silicon dioxide advances into the silicon wafer, while also growing into the ambient. The final pattern can either have a Gaussian [8] or a Lorentzian [18] profile, with a desired height and width, presented as the full width at half maximum (FWHM); the presented simulator provides both distributions. The simulation of local nano-oxidation is performed using a Monte Carlo technique: a desired number of particles is randomly distributed, using a Gaussian or Lorentzian distribution, around the tip of the needle. When a particle reaches the oxide-silicon interface, the oxide is expanded at a velocity which depends on the applied bias voltage and pulse time. The oxide-silicon interface advances into the wafer, while the oxide surface grows into the ambient. The result, after the full pulse time, is a localized oxide dot which has the height and width suggested by the implemented model. The advantage of simulations in this environment is the ease with whitch further lithographic steps [19] can be performed.

2.2. STM Method

When operating in STM mode, a constant tunneling current is present, which exponentially dependens on the distance between the microscope tip and the conductive surface [9]. In order to simulate oxidation patterns using STM, the model presented in [15] was implemented. The equation which governs the height of the grown oxide is given in [15] as

$$h\left(t,V\right)=\frac{V}{E_0}\ln\left(\frac{RE_0t}{V}+1\right), \qquad (1)$$

where t is the pulse time, V is the bias voltage, and E_0 and R are fitting parameters, with E_0=45V/nm and R=1.5×10^3nm/s. At high voltages and long pulse times, the height deviates significantly due to the formation of a water bridge between the tip and the wafer [15]. The simulator is adjusted to handle this behavior by increasing R to 2.3×10^7nm/s and introducing a series voltage drop [15]. Figure 1 shows the measured and modeled heights for this process.

The simulator also requires a model for the FWHM of the grown oxide in order to know how to distribute the accelerated particles. The work presented in [15] provides some measured results, shown in Figure 2. An empirical equation developed to fit the measured results is

$$w\left(t,V\right)=w_0\left(V\right)+w_1\left(V\right)\ln\left(\frac{7t}{V}\right), \qquad (2)$$

where $w_0\left(V\right)=\frac{R}{E_0}\left(1+\frac{1}{2}V\right)$ and $w_1\left(V\right)=2.9V$. The developed model suggests that the width of the profile has a logarithmic dependence on the pulse time and inverse logarithmic dependence on the applied voltage, similar to the dependence observed from the oxide height model. Once again, the model had to be adjusted for the case when a high voltage and long pulse times are applied.

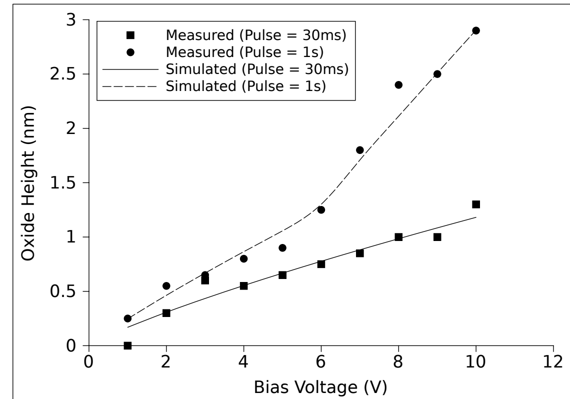

Fig. 1. Height of the oxide as a function of the applied voltage bias, as presented in [15] and implemented in the presented simulator.

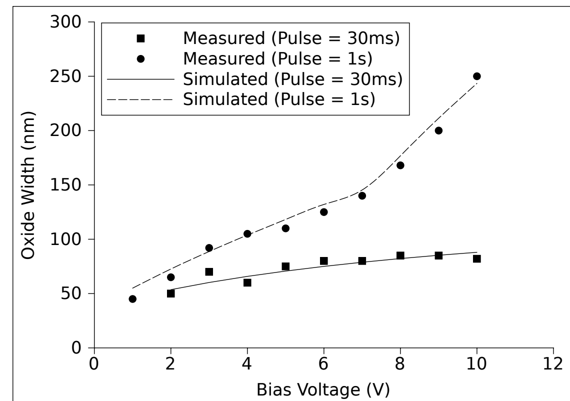

Fig. 2. FWHM of the oxide as a function of the applied voltage bias. Measurements are from [15], while the simulations are from Equation 2.

2.3. AFM Method

When operating in NCM-AFM mode, the formation of a field-induced liquid bridge is required in order to provide oxyanions (OH^-, O^-), used to form the oxide. The liquid bridge also limits the lateral extensions of the region to be oxidized [14]. The model, implemented in the process simulator, is described in [14], where it is suggested that the width and height of a produced pattern have a linear dependence on the applied bias voltage, while a logarithmic dependence exists for the pulse duration.

The empirical equation which governs the height of the oxide dot, produced using NCM-AFM mode, and presented in [14] is

$$h\left(t,V\right)=h_0\left(V\right)+h_1\left(V\right)\ln\left(t\right), \tag{3}$$

where $h_0\left(V\right)=-2.1+0.5V-0.006V^2$ and $h_1\left(V\right)=0.1+0.03V-0.0005V^2$. Similarly, the equation which governs the width of the oxide dot, represented as the FWHM is [14]

$$w\left(t,V\right)=w_0\left(V\right)+w_1\left(V\right)\ln\left(t\right), \tag{4}$$

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. The dependence behavior of the oxide height and width with respect to the bias voltage and pulse time is evidenced in Figure 3, where Equation 3 and Equation 4 are represented graphically.

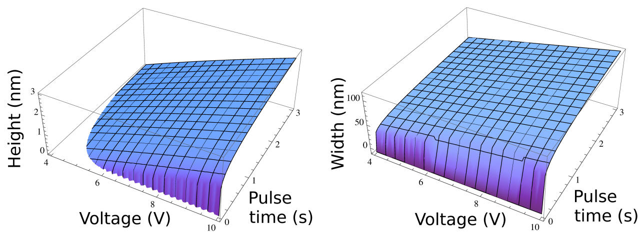

Fig. 3. Height and width of the oxide as a function of the applied voltage bias and pulse time.

3. SAMPLE SIMULATIONS

The simulations were performed using the models described in Section 2. The user can choose whether the pattern should exhibit the properties of a Gaussian curve or a Lorentzian curve. The differences between the two options are shown in Figure 4 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 2.1 a height of 1nm and a width of 5.6nm are expected.

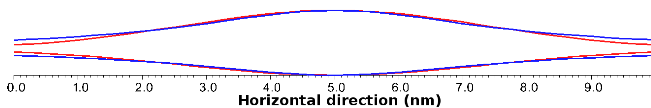

Fig. 4. Cross-section of the oxide pattern when using Gaussian (red) distribution and Lorentzian (blue) distribution. Voltage=20V, Pulse time=0.125ms.

Figure 4 shows the differences in the resulting oxide profile when a Gaussian or Lorentzian distribution is used as the basis for the simulation. Both simulations were performed with the same bias voltage and pulse times. The resulting profile shows that both simulations possess the same height and FWHM, which are 1nm and 5.6nm, respectively.

The results for STM and AFM are shown in Figure 5 and Figure 6, respectively. The top (red) surface represents the interface between the oxide and the ambient, while the bottom (blue) surface represents the interface between the oxide and the silicon substrate.

3.1. STM Simulation

The experimental results used as a basis for the STM simulation are from [15]. The experiment was performed on 10Ωcm p-type silicon wafers passivated with hydrogen. The bias voltage was applied to a positively charged silicon ultralever tip at 95% relative humidity.

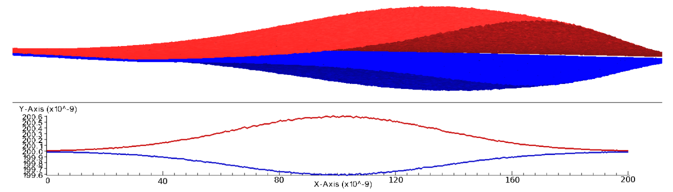

Fig. 5. STM simulation: bias voltage is 8V and pulse width is 33ms. Top surface (red) is the oxide-ambient interface, while the bottom surface (blue) is the oxide-silicon interface.

An oxide height of 1nm was achieved by simulating STM with an applied bias voltage of 8V for a pulse time of 33ms. This shows that the simulator performs in accordance with the measured results from [15] and the model described in Section 2. The width of the oxide achieved in the simulation is 85nm, which matches the experimental results and the presented model.

3.2. AFM Simulation

The experimental results used as a basis for the NCM-AFM simulation are from [14]. The experiments were carried out using a positively charged silicon cantilever with average force constant (k_c) and resonance frequency (f_0) at 34N/m and 330kHz, respectively. The silicon samples were p-type with a 14 Ωcm resistivity.

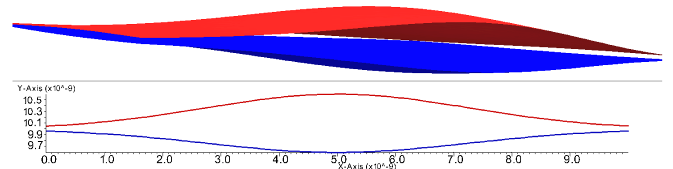

Fig. 6. AFM simulation: bias voltage is 20V and pulse width is 0.125ms. Top surface (red) is the oxide-ambient interface, while the bottom surface (blue) is the oxide-silicon interface.

An oxide height of 1nm was achieved by simulating AFM with an applied bias voltage of 20V for a pulse time of 0.125ms. The simulator performs in accordance with the measured results from [14] and the model described in Section 2. The width of the oxide achieved in the simulation is 5.6nm, which matches the experimental results and the model from [14].

4. CONCLUSION

A simulator for the local anodic oxidation of silicon surfaces is presented for STM and NCM-AFM. The models used were developed to match experimental results. The results of sample simulations showed the ability to grow an oxide 1nm thick. The simulations can easily be incorporated with further processing steps such as mask photolithography, etching, and deposition. An empirical model for the width of the STM-grown oxide is also presented and implemented in the simulator.

5. REFERENCES

[1] G. Binning and H. Rohrer, "Surface Studies by STM," *Physical Review Letters*, 1982.

[2] G. Binning, C. F. Quate, and C. Gerber, "Atomic Force Microscopy," *Physical Review Letters*, p. 930, 1986.

[3] Q. Tang, S.-Q. Shi, and L. Zhou, "Nanofabrication with Atomic Force Microscopy," *Journal of Nanoscience and Nanotechnology*, vol. 4, no. 8, pp. 948–963, Nov 2004.

[4] J.A. Dagata, J. Schneir, H.H. Harary, C.J. Evans, M.T. Postek, and J. Bennett, "Modification of Hydrogen-Passivated Silicon by a Scanning Tunneling Microscope Operating in Air," *Applied Physics Letters*, vol. 56, pp. 2001–2003, May 1990.

[5] P. Avouris, T. Hertel, and R. Martel, "Atomic Force Microscope Tip-Induced Local Oxidation of Silicon: Kinetics, Mechanism, and Nanofabrication," *Applied Physics Letters*, vol. 71, pp. 285–287, Jul 1997.

[6] R.V. Martínez, N.S. Losilla, J. Martinez, Y. Huttel, and R. Garcia, "Patterning Polymeric Structures with 2nm Resolution at 3nm Half Pitch in Ambient Conditions," *Nano Letters*, vol. 7, pp. 1846–1850, Jul 2007.

[7] G. Qin and C. Cai, "Sub-10-nm Patterning of Oligo(Ethylene Glycol) Monolayers on Silicon Surfaces via Local Oxidation Using a Conductive Atomic Force Microscope," *Nanotechnology*, vol. 20, no. 35, pp. 355306, 2009.

[8] A. Notargiacomo and A.A. Tseng, "Assembling Uniform Oxide Lines and Layers by Overlapping Dots and Lines Using AFM Local Oxidation," in *Nanotechnology, 9th IEEE Conference on*, Jul 2009, pp. 907–910.

[9] P.A. Fontaine, E. Dubois, and D. Stiévenard, "Characterization of Scanning Tunneling Microscopy and Atomic Force Microscopy-Based Techniques for Nanolithography on Hydrogen-Passivated Silicon," *Journal of Applied Physics*, vol. 84, no. 4, pp. 1776–1781, 1998.

[10] L. Weng, L. Zhang, Y.P. Chen, and L.P. Rokhinson, "AFM Local Oxidation Nanolithography of Graphene," *Applied Physics Letters*, vol. 93, 2008.

[11] P. Avouris, Y.M. Lin, F. Xia, T. Mueller, D.B. Farmer, C. Dimitrakopoulos, and A. Grill, "Graphene-Based Fast Electronics and Optoelectronics," in *Device Research Conference (DRC)*, Jun 2010, pp. 205–206.

[12] D. Stiévenard, P.A. Fontaine, and E. Dubois, "Nanooxidation Using a Scanning Probe Microscope: An Analytical Model Based on Field Induced Oxidation," *Applied Physics Letters*, vol. 70, pp. 3272–3274, Jun 1997.

[13] P. Avouris, R. Martel, T. Hertel, and R. Sandstrom, "AFM-Tip-Induced and Current-Induced Local Oxidation of Silicon and Metals," *Applied Physics A: Materials Science & Processing*, vol. 66, pp. 659–667, 1998.

[14] 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.

[15] E. S. Snow, G. G. Jernigan, and P. M. Campbell, "The Kinetics and Mechanism of Scanned Probe Oxidation of Si," *Applied Physics Letters*, vol. 76, no. 13, pp. 1782–1784, 2000.

[16] J. A. Dagata, F. Perez-Murano, G. Abadal, K. Morimoto, T. Inoue, J. Itoh, and H. Yokoyama, "Predictive Model for Scanned Probe Oxidation Kinetics," *Applied Physics Letters*, vol. 76, no. 19, pp. 2710–2712, 2000.

[17] M.S. Johannes, D.G. Cole, and R.L. Clark, "Three-Dimensional Design and Replication of Silicon Oxide Nanostructures Using an Atomic Force Microscope," *Nanotechnology*, vol. 18, pp. 345304, Aug 2007.

[18] J.C. Huang, C.-L. Tsai, and A. A. Tseng, "The Influence of the Bias Type, Doping Condition and Pattern Geometry on AFM Tip-Induced Local Oxidation," *Journal of the Chinese Institute of Engineers*, vol. 33, no. 1, pp. 55–61, 2010.

[19] O Ertl and S. Selberherr, "A Fast Level Set Framework for Large Three-Dimensional Topography Simulations," *Computer Physics Communications*, vol. 180, no. 8, pp. 1242–1250, 2009.