Analysis on 3-Dimensional spatial electric field of AFM based anodic oxidation

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Abstract—Atomic force microscope (AFM) based anodic oxidation is an important method to fabricate nano-structures and nano-devices. To realize precise fabrication, electric field between AFM tip and substrate should be under precise control. For precise control of the electric field, a necessary topic is to find out the distribution of the spatial electric field and the relationship between the electric field and parameters. By theoretical analysis we simulated the spatial distribution of the tip/substrate electric field and analyzed the relationship between the electric field and parameters, which were verified by experiments. Our work can provide theoretic support for electric field assisted nanofabrication.

Keywords-AFM; electrical fabrication; anodic oxidation

I. INTRODUCTION

In 1993, H. C. Day first reported anodic oxidation with STM[1]. Since then researchers have investigated AFM based anodic oxidation. Just one year later, E. S. Snow presented a method for fabricating Si nano-structures with an air-operated AFM[2]. As regards mechanism, P. Avouris examined kinetics and mechanism of AFM based anodic oxidation in 1997[3]. To improve anodic oxidation method B. Legrand proposed an original way which could both increase the reliability and improve the nanolithography resolution in 1999[4]; X.-D. Hu analyzed current of dynamic electric field induced oxidation nanofabrication with AFM in 2010[5].

To improve the reliability and resolution of anodic oxidation, we focused on the tip/substrate 3-dimensional spatial electric field in this paper. First we constructed the simulation model for the spatial electric field and attained its distribution. The vertical section of the spatial electric field showed that the electric field was mostly confined within the water meniscus at the tip-substrate junction. J. A. Dagata indicated that product ion concentrations associated with the water meniscus[6] and R. Garcia realized to confine the oxidation of silicon surfaces with a non-contact AFM by controlling the nanometer-size water bridges[7]. Our simulation coincided with Dagata and Garcia. The horizontal section showed that the electric field wears off from inside out. Next the electric field variation under the existence of nano-oxide line was simulated. After that the relationship between the electric field and parameters was analyzed. Ten simulations were carried out with tip-substrate voltage varying from 1V to 10V and illustrated a linear relationship with the voltage. Another ten simulations with tip/substrate separation varying from 1nm to 10nm confirmed an exponential relationship with the tip/substrate separation. Then the impact of the water meniscus on the electric field was discussed. However the heights of the water films on the substrate and the tip surface had a slight impact on the electric field deducing from our simulation. Next two groups of nano-dots were fabricated on Si substrate to illustrate our simulations. One group was made under the same experimental conditions except different tip-substrate separations and the other group was fabricated under the same conditions except different voltages. The variation trends of the nano-dots coincided with our simulations. At last a group of nano-lines was fabricated on Si substrate under instructions of our simulation. The mean value of the heights of these lines was 1.64nm and the variance was 0.13nm². The data showed that the lines were of good repetition. In brief, our works can help to plan procedure for fabricating nano-transistors or nano-masks by anodic oxidation.

II. SIMULATION MODEL

Gomer R set up a model for STM tip electric field in 1986[8]. STM Tip was equivalent to a sphere in the model, as shown in Fig. 1(a). Gomer R also deduced an equation by using image potentials shown as (1) to calculate the electric field on substrate surface. \(E(r)\) represented Electric field intensity at point A in fig. 1(a). \(V, D, R, r\) were as shown in Fig. 1(a).

\[
E(r) = \frac{V}{D} \left[1 + \left(\frac{r}{R + D}\right)^2\right]^{-\frac{3}{2}}
\]

AFM has similar structure with STM. However AFM works in air and the tip is connected with the substrate by a meniscus[9], as shown in fig. 1(b). The existence of the meniscus...
makes it hard to build up a formula to calculate the electric field on the substrate.

We adopted simulation method to study the spatial distribution of the electric field between AFM tip and substrate. Electric field in space rather than just that on the substrate surface could be studied through simulation method. Further more electric field variation when parameters changed could be discussed by simulation. According to Poisson's equation, available mathematic model for space electric field was shown as (2):

\[
-\nabla \cdot [(\varepsilon / T + \sigma)\nabla V - (J' + P / T)] = \rho / T
\]

Among (2), \(\nabla\) is the Hamiltonian operator, \(\varepsilon\) is the dielectric constant, \(\sigma\) is the conductivity, \(J'\) is the external current density, \(\rho\) is the space charge density, \(P\) is the polarization vector, and \(T\) is the time step.

Equation (2) was broken down into two parts in the simulation software we used in order to reduce difficulty of solving. The first part was shown as (3). This part was used to calculate electric field within the thin water film, as shown in Fig. 1(b). The other part was shown as (4) and was used to calculate electric field in the air sub-domain, as shown in fig. 1(b).

\[
-\nabla \cdot (\sigma \nabla V - J') = Q
\]

\[
-\nabla \cdot \varepsilon \varepsilon_n \nabla V = \rho
\]

The geometric model of AFM tip was based on NSC15/Ti-Pt, which was a conductive tip from MikroMasch Company coated with 15nm Ti first and then 10nm Pt. The tip was equivalent to a cone with a sphere on the end point, as shown in Fig. 1(b). The height of the water film \(h\) was a variable in the simulation. Substrate was simplified to a round panel with a radius as long as 500nm. A bigger radius was proved to be useless to improve simulation results because electric filed gathered closely around the peak point of AFM tip. The height of the panel was ignorable because electric field inside the panel was zero.

III. SIMULATION ANALYSIS

A. Simulation Results

The spatial distribution of the electric field was shown in Fig. 2. Fig. 2 was simulation results under conditions that \(h\) equaled 5nm, tip-sample separation \(D\) equaled 5nm, and tip bias \(V\) equaled 10V. Only electric field distribution in the water film was presented and that in the air was blocked because electric field in the air was relatively less important.

The coordinate system of Fig. 2 was set as below. Y-axis was along the central axis of the tip. XZ plane paralleled to the substrate surface. The origin was located at the end point of the tip. Cut the Fig. 2(a) along Y-axis, and the vertical section of the electric field could be derived, shown as Fig. 2(b). As we could see from Fig. 2(b), the electric field was symmetrical about Y-axis, and the farer from Y-axis, the lower the electric field was. In the meniscus the electric field displayed a funnel-shape and decreased from top to down. Fig. 2(c) was the horizontal section of Fig. 2(a). The electric field spread in round-shape and decreased outward from the center as shown in Fig. 2(c).

Electric field on a line across the center of substrate surface could represent that on the whole surface as the electric field on the substrate surface was symmetrical about the center. Every one of the four curves in Fig. 3 represented electric field on the substrate surface. X-axis was distance from the center and Y-axis was normal value of electric field in Fig. 3. Curve 1 was calculated by (1). Curve 2 was simulation result assuming the tip was a sphere and without considering the water film. Curve 1 and Curve 2 were obtained under same geometry models and physical conditions but using different methods, so they were supposed to match with each other. Actually they were not, as shown in Fig. 3. On possible reason was that in the derivation of (1) with image potential...
method the tip was equivalent to a sphere first and then assumed as a point charge which was located in the center of the sphere. Actually the position of the point charge was a little below the center. The assumption was made to avoid solving high-order equation. Curve 3 was simulation result on conditions that AFM tip was equivalent to a cone and ignore water films over tip and substrate. Curve 2 and curve 3 were derived under same conditions except the shape of the tip. A cone-shape was closer to the real shape of AFM tip. The difference between curve 2 and curve 3 reflected the effect of the tip-shapes on the electric field. Curve 4 was derived considering the water film and the tip as a cone. The difference between curve 3 and curve 4 reflected the effect of the water film on the electric field. Under consideration of water film, the electric field further concentrated to center.

Among anodic oxidation processing, already generated oxide might disturb the existed electric field. Fig. 4 showed the electric field distribution in the presence of line-shape oxide as high as 2nm. Comparing Fig. 4 with Fig. 3(b), the electric field in Fig. 4 was bigger.

B. Electric field under different tip bias

The electric field between the tip and substrate is aroused by tip bias voltage, so the bias has a significant impact on the electric field. When the water film was as thick as 5nm and tip-substrate distance was 5nm, tip bias varied from 1V to 10V, thus ten corresponding distributions of the electric field were obtained, as shown in Fig. 5(a). Image 1 was electric field when tip bias was 1V, and so on. The bigger the bias voltage was, the stronger the electric field was, as we can see from Fig. 5(a). When the bias voltage was under 6V, the magnitude of the electric field was less than $10^9$V/m, which was the threshold voltage for anodic oxidation. For precious investigation of the electric field on substrate surface, image data of Fig. 5(a) were exported and data on a line across center of substrate surface were picked up to form ten curves as shown in Fig. 5(b). Curve 1 in Fig. 5(b) corresponded to image 1 in Fig. 5(a). Curve 2 in Fig. 5(b) corresponded to image 2 in Fig. 5(a), and so on. From Fig. 5(b) we could conclude that the peak value of the substrate surface electric field located at the center, and the electric field was symmetrical about the center. The electric field on a certain point of the substrate surface was linear with the tip bias, as shown in Fig. 5(c). Six points on the substrate surface were chosen. Point 1 corresponded to curve 1 in Fig. 5(c) and located on the center. Point 2 was 10nm away from the center, and so on.

C. Electric field under different tip-substrate seperation

Tip-substrate separation is another important factor to affect the electric field. When tip bias was kept as 10V and water-film height was kept as 5nm, tip-substrate separation varied form 1nm to 10 nm, thus a collection of ten images was obtained as shown in Fig. 6(a). Image 1 was electric field distribution when tip-substrate distance was 1nm, and so on. The smaller the separation was, the stronger the electric field was, as we could see from Fig. 6(a). When the separation was over 9nm, the magnitude of the electric field was less than...
10^9 V/m, which was the threshold voltage for anodic oxidation. For precious investigation of the electric field on substrate surface, image data of Fig. 6(a) were exported and data on a line across center of substrate surface were picked up to form ten curves as shown in Fig. 6(b). Curve 1 in Fig. 6(b) corresponded to image 1 in Fig. 6(a). Curve 2 in Fig. 6(b) corresponded to image 2 in Fig. 6(a), and so on. From Fig. 6(b) we could also conclude that the peak value of the substrate surface electric field located at the center, and the electric field is symmetrical about the center. The electric field of a certain point on the substrate surface was non-linear with the separation, as shown in Fig. 6(c). Also six points on the substrate surface were chosen. Point 1 corresponded to curve 1 in Fig. 6(c) and located on the center. Point 2 was 10nm away from the center, and so on.

D. Electric field under different heights of water film

Both AFM tip and substrate was cover by water films. The height of the water film was related to the humidity of the air. We simulated variation of the electric field under different water-film heights. In Fig. 7 the difference between electric fields with and without water film had been discussed. The impact of the water-film height on the electric field was going to be discussed in this section. Kept the tip bias 10V constantly and tip-substrate separation 5nm and varied the height of the water film from 1nm to 10nm, thus a cluster of curves was obtained as shown in Fig. 7. Curve 1 represented the electric field on the substrate surface when the water film height was 1nm, and so on. The water film height only played a role in the area approximately 25nm far away from the substrate surface center. Within 25nm, the electric field kept constant no matter what was the height. One possible reason was the water film over the tip and that over the substrate connected with each other to form a water bridge. When the water film varied the width of the bridge changed. The electric field was strong mostly in the bridge. Outside the bridge the electric field decreased rapidly to zero. The boundary between the bridge and the air constrained the electric field inside the bridge. So when the water bridge grew broader, the electric field reached out.

IV. EXPERIMENTAL RESULTS

Experiments fabricating nano-dots and nano-lines on silicon substrate have been conducted for analyzing relations between results of electric field simulation and nano-structure fabrication. Fig. 8(a) shows results of six nano-dots fabricated with two different conditions, and Fig. 9 shows results of nine nano-lines fabricated under the same condition. The six nano-dots in Fig. 8(a) are divided into two groups. Group 1 included Dots D1, D2 and D3, which were fabricated under same tip bias but different tip-substrate distance. Dots D4, D5 and D6 were group 2, which were fabricated under different tip bias while tip-substrate distance was kept constant. Take D1 for example, the mark on the upper left corner of D1 (10V, 5nm) means D1 was fabricated under 10V tip bias and 5nm tip-substrate distance. The time period of tip bias was 1 second for all the six nano-dots.

Fig. 8(b) showed the widths and heights of dots D1 to D6. The higher curve in Fig. 8(b) was height values on the line across D1, D2 and D3 in Fig. 8(a). The lower curve in Fig. 8(b) was height values on the line across D4, D5 and D6 in Fig. 8(a). Dot D1 was about 3.7nm high. The heights of dots D2 and D3 were very close. Fig. 8(b) approximately represented that the heights of D1, D2 and D3 had an inverse relationship
with tip-substrate distance and the relationship was nonlinear, while the heights of D4, D5 and D6 were proportional to the tip bias.

However the widths grew boarder from D1 to D3 while the widths grew narrower from D4 to D6. The widths of these nano-dots were not simply proportional to the amplitude of the electric field. The simulation results of electric field when fabricating D1 to D6 was put on in Fig. 8(c) to discuss the relationship between the shapes of D1 to D6 and the electric field. The curve D1 in Fig. 8(c) represented the electric field under which dot D1 was fabricated, and so on. D3 and D4 were fabricated under same parameters. However the experimental results were different. One possible reason was the substrate environment of group 2 differed from that of group 1. Furthermore R1 was corresponding to R2. Take D1 for example, R1 of D1 was smallest in group 1, correspondingly R2 was the smallest one in group 1.

Table 1 recorded the heights and widths of the experimental nano-dots in Fig. 8(a), the amplitude of electric field simulation results and the width within which the simulation result was over $10^9$V/m. From table 1 we could see that when R1 was bigger, the dot was wider. This was true inside group 1 and group 2 respectively, but not so between the two groups. One possible explanation was the substrate environment of group 2 differed from that of group 1. Furthermore R1 was corresponding to R2. Take D1 for example, R1 of D1 was smallest in group 1, correspondingly R2 was the smallest one in group 1.

Fig. 9 showed nine nano-lines fabricated on silicon substrate under same parameters. The nine nano-lines were made in one
fabrication. The AFM tip was 5nm high from substrate and moved from up to down by 200nm/s after a 12V bias loaded to AFM tip. After a nano-line was fabricated, the above process was repeated automatically until the last line was finished. The mean value of the heights of these lines is 1.64nm and the variance is 0.13nm² from three scanning measurements crossing the lines. The data and scanned image show that the lines are of good repetition.

V. CONCLUSION

We studied the electric field caused by the tip bias of AFM by simulation and analyzed the relationship between the electric field and parameters such as tip bias, tip-substrate distance and water-film height. Variation of electric field under different tip bias and tip-substrate distance was discussed. The impact of water films over tip and substrate was studied. Then some simple nano-structures were fabricated to verify simulation result. Experimental results approximately meet simulation results. So our simulation can provide helpful instruction for anodic oxidation processing.

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