PROBE SHAPE RECOVERY IN SCANNING PROBE MICROSCOPY

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ABSTRACT

This paper presents an algorithm for recovering, *in situ*, the shape of the probe used in a scanning probe microscope. The inputs to the algorithm are the image of a reference surface and the known shape of the reference surface. The output is a depth map representing the three dimensional shape of the probe. This recovered probe shape can be used to restore images of unknown surfaces. A method for determining certainty of recovery is also presented.

1 INTRODUCTION

Scanning probe microscopy (SPM), which includes techniques such as scanning tunneling microscopy (STM) and scanning force microscopy (SFM), is being recognized as a powerful method for obtaining three dimensional digital images of surfaces at submicron resolution [6]. Application areas of SPM include inspection and three-dimensional metrology of semiconductor wafers, high resolution imaging of surface topography in Chemistry and Materials Science, and imaging of individual cells in Biology.

Imaging in SPM is performed by scanning the sample surface, in a contact or non-contact mode, by means of a probe of micron or sub-micron dimensions. The probe used for scanning is a vital component of a scanning probe microscope and characterization of its shape is important. The images produced in SPM are invariably distorted due to the non-ideal geometry of the scanning probe. Restoration methods can be used to recover the true surface from the SPM image, given the shape of the probe used for scanning, as we have described elsewhere [4, 5]. Moreover, the shape of the probe may vary over time. Parts of the probe surface may be abraded due to the contact with the sample. Hence it is important to characterize the shape of the probe from time to time.

The method most commonly used to determine probe shape is scanning electron microscopy (SEM). This method requires that the probe be dismounted from the microscope and imaged. This method is cumbersome and the probe may be damaged in the process. Another disadvantage of this method is that the probe surface may have to be metal-coated before imaging. The probe may no longer be functional after such coating. Finally, SEM gives only a two-dimensional shape of the probe. Hence, it remains hard to determine the three-dimensional shape which is required for the restoration algorithms.

Gallarda and Jain [1] suggested that the probe shape can be recovered from an image by eroding the image with the known shape of the true surface. But they did not justify their claim and showed no experimental results. Grigg *et al* [3] also suggested that images of known structures can be used for characterization of probe shape. They show results of probe shape recovery with STM. They use the sidewall profiles of images of square pillars to estimate the shape of the probe. They give no computational algorithm. They manually segment out the the sidewall profiles and manually combine them. They use this method to obtain a two-dimensional view of the probe shape.

In this paper we show that the shape of the probe may be recovered *in situ* from the distortion caused by the probe on the image of a known surface. We develop an algorithm to recover the shape of a probe from a contact mode image of a reference surface obtained using the probe. We also develop a method to indicate the certainty of recovery of probe shape. The main advantages of our algorithm are that it gives a three-dimensional representation of the probe shape, and does not require the probe to be dismounted from the microscope. The method for probe shape recovery is an important calibration step for a scanning probe microscope.

2 PROBE SHAPE RECOVERY

Probe shape recovery can be based on the constraints imposed by the imaging process. Two such constraints for contact mode imaging were stated in [4]. One of these constraints is
$\forall(x_1, y_1), (x_2, y_2) \epsilon D_I$

$$I(x_2, y_2) + P_{x_2,y_2}(x_1, y_1) \geq S(x_1, y_1) \quad (1)$$

Here, I denotes the image function, S the true surface function, P the probe shape function. $f_{a,b}$ is used to denote the translation of function f by (a, b). D_f is used to denote the domain of function f. The constraint states that during imaging, the height of every point on the probe is greater than the height of the corresponding point on the true surface.

Using the definition of the translation of a function, the constraint in 1 can be rewritten as
$\forall(x, y) \epsilon D_P, (x_2, y_2) \epsilon D_I$

$$P(x, y) \geq S(x + x_2, y + y_2) - I(x_2, y_2) \quad (2)$$

Or,
$\forall(x, y) \epsilon D_P$

$$P(x, y) \geq max_{(x_2,y_2)\epsilon D_I} S(x + x_2, y + y_2) - I(x_2, y_2) \quad (3)$$

Therefore, an estimate of the probe shape can be given as
$\forall(x, y) \epsilon D_P$

$$EP(x, y) = max_{(x_2,y_2)\epsilon D_I} S(x + x_2, y + y_2) - I(x_2, y_2) \quad (4)$$

Or,
$\forall(x, y) \epsilon D_P$

$$EP(x, y) = max_{(x_2,y_2)\epsilon D_I} S(x + x_2, y + y_2) - I(x_2, y_2) \quad (5)$$

Or,
$\forall(x, y) \epsilon D_P$

$$EP(x, y) = max_{(x_2,y_2)\epsilon D_I} S_{-x_2,-y_2}(x, y) + I^{\wedge}(-x_2, -y_2) \quad (6)$$

where

$$I^{\wedge}(x, y) = -I(-x, -y) \quad (7)$$

is the reflection of the image function about the origin. Equation 6 may be rewritten as
$\forall(x, y) \epsilon D_P$

$$EP(x, y) = max_{(x_2,y_2)\epsilon D_I} S_{x_2,y_2}(x, y) + I^{\wedge}(x_2, y_2) \quad (8)$$

Or, using the definition of gray scale morphological dilation [2], we have

$$EP(x, y) = [I^{\wedge} \oplus S](x, y) \quad (9)$$

Equation 9 suggests that an estimate of the true probe shape can be obtained from an image obtained using the probe if the true surface is known. The probe shape estimate is given by the gray scale morphological dilation of the reflection of the image function about the origin with the shape of the true surface. Note that this result is quite different from that suggested in [1]. One great advantage of this equation is that it does not require that we explicitly identify the distorted regions in the image. The dilation based method automatically gets the estimate of the probe shape given the image and the surface. This is unlike the method of Grigg *et al* [3] who manually determine the portions of the image that are distorted. Clearly, the greatest demand made by this algorithm is that the true surface should be known. Besides, the true surface shape and the image should be aligned to each other for the method to work. Even if the true shape of a calibration pattern is known, alignment poses a difficulty. A solution would be to use a matching algorithm to match the model shape with the image in order to align them. Future research will have to address this issue.

3 CERTAINTY OF RECOVERY

It is important to determine where the probe recovery is certain. For this, we once again use the constraints imposed by the imaging process. A second constraint imposed by the imaging process is
$\forall(x_2, y_2) \epsilon D_I, \exists(x_1, y_1) \epsilon D_S, (x, y) \epsilon D_P$ such that

$$P_{x_2,y_2}(x, y) = S(x_1, y_1) - I(x_2, y_2) \quad (10)$$

where

$$(x, y) = (x_1 - x_2, y_1 - y_2) \quad (11)$$

This constraint states that every point on the image corresponds to the height of some point on the probe when the probe touches some point on the true surface.

The constraint equation can be rewritten as
$\forall(x_2, y_2) \epsilon D_I, \exists(x, y) \epsilon D_P$ such that

$$P_{x_2,y_2}(x, y) = S(x + x_2, y + y_2) - I(x_2, y_2) \quad (12)$$

From equations 3 and 12 we have,
$\forall(x_2, y_2) \epsilon D_I, \exists(x, y) \epsilon D_P$ such that

$$\begin{aligned} P(x, y) &= max_{(x_2,y_2)\epsilon D_I} S(x + x_2, y + y_2) - I(x_2, y_2) \\ &= EP(x, y) \end{aligned} \quad (13)$$

Therefore, for any $(x_2, y_2) \epsilon D_I, \exists(x, y) \epsilon D_P$ such that

$$P(x, y) = EP(x, y) \quad (14)$$

and

$$I(x_2, y_2) = S(x + x_2, y + y_2) - EP(x, y) \qquad (15)$$

Therefore, if for some $(x_2, y_2)\epsilon D_I$, there exists only one (x, y) which satisfies equation 15 we have for such (x, y) that $EP(x, y)$ necessarily equals $P(x, y)$. In other words,

$EP(x, y) = P(x, y)$
if $\exists(x_2, y_2)\epsilon D_I$ such that
$I(x_2, y_2) = S(x_2 + x, y_2 + y) - EP(x, y)$
and
$\forall(x_a, y_a), (x_a, y_a) \neq (x, y)$
$I(x_2, y_2) \neq S(x_2 + x_a, y_2 + y_a) - EP(x_a, y_a)$

This is a condition that can be used to check the certainty of recovery of any point on the estimated probe shape. Thus, not only can we estimate the probe shape but also indicate where the estimation is certain.

4 EXPERIMENTAL RESULTS

Several experiments were run to test the efficacy of the probe shape recovery algorithm. Here we present results with a pyramidal probe used to scan a cylindrical structure. Figure 1 shows a scanning electron microscope (SEM) image of a pyramidal probe. Figure 2 shows the scanning electron microscope image of a microfabricated cylindrical structure on a silicon wafer. The diameter of the cylinder is 4 microns and its height is 1.3 microns. Figure 3 shows an atomic force microscope (AFM) image of the fabricated cylinder. Figure 4 shows the probe shape recovered from the image of the cylinder. This was obtained by providing a model of the cylinder along with the image of the cylinder to the probe shape recovery algorithm. It is seen that the dimensions of the probe correspond to those of the SEM image of the pyramidal probe. The probe shape is recovered up to the height of the cylinder. It is seen that the probe is tilted. This is due to the actual tilt of the probe in the AFM. Thus, the recovery algorithm gives a true *in situ* picture of the probe shape including the tilt of the probe.

5 Conclusion

We have presented an algorithm based on gray scale morphological dilation for *in situ* characterization of probe shape in SPM. We have also developed a method for indicating certainty of recovery. A significant issue in recovery is matching the model of the calibration pattern with the actual image. This is an issue that needs to be addressed in our future research. Another important issue is the determination of the appropriate calibration pattern for recovering a particular class of probe shapes. Our experiments indicate that a cylindrical pattern is useful for a wide variety of probe shapes.

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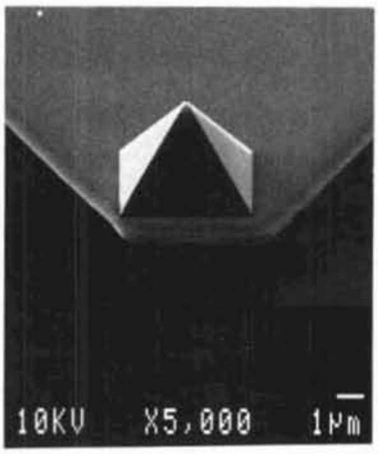

Figure 1: SEM image of pyramidal probe

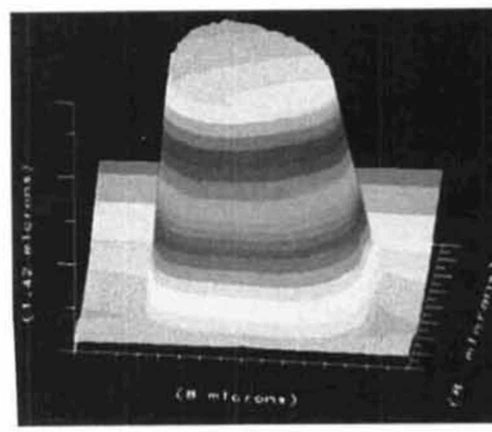

Figure 3: AFM image of cylinder

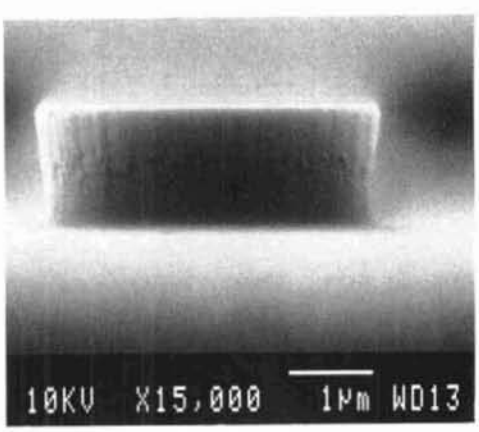

Figure 2: SEM image of fabricated cylinder

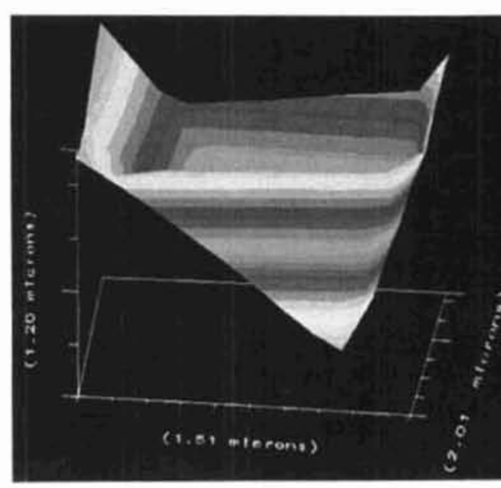

Figure 4: Recovered probe shape