Global Shape Reconstruction of the Bended AFM Cantilever

Yangjie Wei, Chengdong Wu, Zaili Dong, and Zhu Liu

Abstract—Principle of atomic force microscope (AFM) is on the basis of cantilever’s deflection. However, up to now, there are still no effective methods to model the cantilever’s deflection with high precision, which will usually result in a poor measurement accuracy of AFM and has greatly limited further applications of AFM in more different fields. Thus, a global shape from defocus method, which is only based on a single vision sensor, is introduced in this paper to reconstruct the bended shape of AFM cantilever. First, the model of the defocus imaging is given using the concepts of relative blurring and diffusion equation. Second, the relationship between the relative blurring and the interested depth information is built with basic imaging formulas. Subsequently, the depth measurement problem is transformed into an optimization issue and an algorithm is designed to compute the deflection of cantilever. Finally, extensive experiments are conducted and results are analyzed to show the feasibility and the effectiveness of the proposed method.

Index Terms—Atomic force microscope (AFM), bended cantilever, shape reconstruction.

I. INTRODUCTION

SINCE atomic force microscope (AFM) was first developed in 1986, it has been widely used in micro/nanomanipulation, and now it is a well-known tool utilized to investigate characteristics of samples on micro/nanometer scale [1]–[4].

Normally, an AFM is composed of two main components: a scanner and an AFM detection system. The scanner houses a piezoelectric transducer, which can physically move a sample in all x-, y-, and z-direction, while the detection system consists of a laser and pair of photodiodes, where the laser generates a spot of light and the photodiodes detect the reflected light by a microfabricated cantilever. The principle of using AFM to measure the height of a sample is as follows: 1) the sample moves in both x- and y-direction under a tip equipped at the end of the cantilever while maintaining the tip in contact with the sample surface; 2) when the height of the sample changes, the cantilever bends with different angles and the position of the reflected light spot, which can be sensed by a circuit whose output voltage is in direct proportion to the position, moves between the two photodiodes; 3) a controller is used to move the cantilever in the z-direction until the output of the circuit is equal to a predefined value that means the bended angle of the cantilever is fixed.

However, the method referred previously is inaccurate in many situations because of several factors. For example, 1) measurement precision of the bended angle is highly related to the direction of the laser and the spot on the cantilever that reflects the light back to the photodiodes. This is because the deflections at different points of the cantilever are different although same force is acted on the tip. But it is difficult to make the direction of the laser time invariant during even one experiment; thus, it is impossible to measure the precise bended degree at each position [5]–[10]; 2) deflection voltage is proportional to the difference signal between two closely spaced photodiodes of the position sensitive detector. In fact, besides height change, many factors, such as viscosity of sample surface, can also influence this difference signal. However, in the interval circuit, deflection voltage is always transformed into the height image, regardless of other factors. Therefore, a method with the ability to directly observe the bended cantilever of AFM on micro/nanometer scale is necessary, since it not only can be used to analyze the measurement error of the preceding methods but also can enlarge applications of AFM greatly.

Nowadays, with precision and resolution improvement of vision sensors, computer vision technique has been used into micro/nanobservation [11], [12]. Compared to other observation methods, requirements of computer vision, such as experiment environment, operation cost, and equipment price, are all lower. Furthermore, with the advantage of direct and real-time observation, optical microscope technologies have been used to image micrometer samples, attain real-time vision feedback, and assist AFM to improve precision, success rate, and efficiency of micro/nano manipulation [9], [13]. Moreover, shape from defocus (SFD), or depth from defocus, has been proved to be an effective shape reconstruction method by using blurring degree of region images and it is widely used in many macroscopic observations [14]–[19]. However, due to wavelength limitation, actual optical microscopes can only observe samples on micrometer scale and many macroscopic algorithms do not satisfy high precision acquisitions.

In this paper, the global shape of a cantilever with different deflection degree is reconstructed with a new SFD method.
The approach that we propose is novel in several ways and achieves optimality without resorting to power spectral density signals or changing the microscope's parameters. It needs a static microscope and two defocused images, and first allows us to observe the real bended shape of the whole cantilever. Furthermore, it is possible to analyze forces at each location in the future.

The contents of this paper are organized as follows. First, in Section II, the defocus imaging model with diffusion equation and relative blurring is introduced. Second, the new shape reconstruction method using one microscope is proposed in Section III. Subsequently, in Section IV, experiment results based on the new method are given. Finally, conclusion is given in Section V.

II. DEFOCUS IMAGING MODEL

In the defocus imaging model, a defocused image can be theoretically considered as the summation of some defocused points, and this process can normally be denoted by the following convolution function:

\[ E(x, y) = I(x, y) * h(x, y) \]  

where \( E(x, y) \) and \( I(x, y) \) are the defocused image and the focused image, respectively, and \( h(x, y) \) is the point spread function.

When the point spread function is approximated by a shift-invariant Gaussian function, the imaging model in (1) can be formulated in terms of the isotropic heat equation

\[
\begin{align*}
\frac{\partial \Delta u}{\partial t} & = \Delta u + \frac{\partial^2 u(x, y, t)}{\partial x^2} + \frac{\partial^2 u(x, y, t)}{\partial y^2}, \\
\Delta u & = \frac{\partial^2 u(x, y, t)}{\partial x^2} + \frac{\partial^2 u(x, y, t)}{\partial y^2}, \\
\end{align*}
\]

where \( \Delta \) is the diffusion coefficient, \( \Delta u = \frac{\partial^2 u(x, y, t)}{\partial x^2} + \frac{\partial^2 u(x, y, t)}{\partial y^2} \) and \( \Delta \) is the point spread function.

If the depth map is an equifocal plane, \( \alpha \) is a constant. Otherwise, \( \alpha \) is a shift variant, and the diffusion equation becomes

\[
\begin{align*}
\frac{\partial \alpha}{\partial t} & = \alpha \Delta u + \nabla \cdot (\alpha \nabla u), \\
\frac{\partial \alpha}{\partial x} & = 0, \\
\end{align*}
\]

where \( \nabla \) and \( \nabla' \) denote the gradient operator and the divergence operator as follows:

\[
\nabla = \left[ \frac{\partial}{\partial x}, \frac{\partial}{\partial y} \right]^T, \quad \nabla' = \frac{\partial}{\partial x} + \frac{\partial}{\partial y}.
\]

It is also easy to verify that the variance \( \sigma^2 \) is related to the diffusion coefficient \( \alpha \) via

\[
\sigma^2 = 2\alpha t.
\]

Suppose there are two images \( E_1(x, y) \) and \( E_2(x, y) \) for two different focus settings; also, \( \sigma_1 < \sigma_2 \) (i.e., \( E_1(x, y) \) is more defocused than \( E_2(x, y) \)); then, \( E_2(x, y) \) can be written as

\[
\begin{align*}
E_2(x, y) & = \int \frac{1}{2\pi\sigma_2^2} \exp \left( -\frac{(x-u)^2+(y-v)^2}{2\sigma_2^2} \right) r(u, v) \, du \, dv \\
& = \int \frac{1}{2\pi\sigma^2} \exp \left( -\frac{(x-u)^2+(y-v)^2}{2\sigma^2} \right) E_1 r(u, v) \, du \, dv
\end{align*}
\]

where \( \Delta \sigma_2 \equiv \sigma_2^2 - \sigma_1^2 \) is called the relative blurring [19]. So, (2) can be written as

\[
\begin{align*}
\frac{\partial u(x, y, t)}{\partial t} & = \alpha \Delta u + \nabla \cdot (\alpha \nabla u), \\
u(x, y, 0) & = E_1(x, y).
\end{align*}
\]

Equation (3) becomes

\[
\begin{align*}
\frac{\partial u(x, y, t)}{\partial t} & = \nabla \cdot (\alpha(x, y) \nabla u(x, y, t)), \\
u(x, y, 0) & = E_1(x, y).
\end{align*}
\]

When the time shifted is \( \Delta t \), the solution of the diffusion equation is \( u(x, y, t) \Delta t \) and \( E_2(x, y) \), and \( \Delta t \) can be defined as

\[
\Delta t = (2t_2 - t_1)a \equiv 2D \Delta t.
\]

Thus, the relation between the relative blurring and the depth map can be denoted as

\[
\Delta \sigma_2 = \gamma (b_2^2 - b_1^2)
\]

where \( \gamma \) is a constant between the blurring radius and the blurring degree, and \( b_i \) (i = 1, 2) is the radius of the blurring round

\[
b = \frac{Dv}{2} \left| \frac{1}{f} - \frac{1}{v} - \frac{1}{s} \right|
\]

where \( s \) denotes the depth of the blurring point and \( D \) denotes the radius of the lens.

III. NEW SHAPE RECONSTRUCTION METHOD

Suppose \( E_1(x, y) \), whose depth map is \( s_1(x, y) \), is the defocused image attained before depth variation, and \( E_2(x, y) \) is another defocused image attained after depth variation. In this section, we will propose a new shape reconstruction method in which the depth map \( s_2(x, y) \) is attained through a depth change \( \Delta s \), and the theory is shown in Fig. 1.

Suppose \( s_0 \) is the focus depth, and \( s_1(x, y) - s_2(x, y) = \Delta s(x, y) \). Based on the diffusion equations in Section II, the
following functions can be given:

\[
\begin{align*}
\dot{u}(x, y, t) &= \nabla \cdot (a(x, y) \nabla u(x, y, t)) \quad t \in (0, \infty) \\
u(x, y, 0) &= E_1(x, y) \\
u(x, y, \Delta t) &= E_2(x, y)
\end{align*}
\]  
(11)

where the relative blurring can be denoted as

\[
\Delta \sigma^2(x, y) = \gamma^2 (b_2^2(x, y) - b_1^2(x, y))
\]

\[
= \frac{\gamma^2 D^2 v^2}{4} \left[ \left( \frac{1}{f} - \frac{1}{v} - \frac{1}{s_2(x, y)} \right)^2 - \left( \frac{1}{f} - \frac{1}{v} - \frac{1}{s_1(x, y)} \right)^2 \right]
\]

\[
= \frac{\gamma^2 D^2 v^2}{4} \left[ \left( \frac{1}{s_0} - \frac{1}{s_2(x, y)} \right)^2 - \left( \frac{1}{s_0} - \frac{1}{s_1(x, y)} \right)^2 \right].
\]  
(12)

Define

\[
k = \frac{4\Delta \sigma^2}{\gamma^2 D^2 v^2} + \left( \frac{1}{s_0} - \frac{1}{s_1(x, y)} \right)^2.
\]

Thus, the desired depth map is

\[
s_2(x, y) = \frac{1}{\left( \frac{1}{s_0} \pm \sqrt{k} \right)}.
\]  
(13)

In real applications, it is reasonable to discuss the following four cases when the distance between the sample and the microscope is becoming shorter.

**A.** $s_1 > s_2 > s_0$

In this case, $s_1(x, y)$ and $s_2(x, y)$ are both larger than $s_0$, and $E_1(x, y)$ is more defocused than $E_2(x, y)$; so, it is a backward diffusion process from $E_1(x, y)$ to $E_2(x, y)$, i.e., the diffusion efficient “$a$” is negative. The theory is shown in Fig. 2 and the final depth can be denoted as

\[
s_2(x, y) = \frac{1}{\left( \frac{1}{s_0} - \sqrt{k} \right)}.
\]  
(14)

**B.** $s_0 > s_1 > s_2$

As shown in Fig. 3, here, $s_1(x, y)$ and $s_2(x, y)$ are both smaller than $s_0$, and $E_1(x, y)$ is less defocused than $E_2(x, y)$; so, it is an afterward diffusion process from $E_1(x, y)$ to $E_2(x, y)$, and the diffusion efficient “$a$” is positive. The final depth can be denoted as

\[
s_2(x, y) = \frac{1}{\left( \frac{1}{s_0} + \sqrt{k} \right)}.
\]  
(15)

**C.** $s_1 > s_0, s_2 < s_0, (s_0 - s_2) < (s_1 - s_0)$

In this case, it is a little more complicated than the first two. $E_1(x, y)$ is more defocused than $E_2(x, y)$, but they are not on the same side of $s_0$. Suppose $s'_2(x, y)$ is the symmetrical depth of $s_2(x, y)$ about $s_0$; this case can be easily transferred from Fig. 4(a) to (b), and the final depth can be denoted as

\[
s_2(x, y) = \frac{1}{\left( \frac{1}{s_0} - \sqrt{k} \right)}.
\]  
(16)

\[
s_2(x, y) = s_0 - (s'_2(x, y) - s_0) = 2s_0 - s'_2(x, y).
\]  
(17)
Here, $E_1(x, y)$ is less defocused than $E_2(x, y)$, and they are not on the same side of $s_0$. Suppose $s'_2(x, y)$ is the symmetrical depth of $s_2(x, y)$ about $s_0$; this case can be transferred from Fig. 5(a) to (b), and the final depth can be denoted as

$$s'_2(x, y) = \frac{1}{(1/s_0 + \sqrt{k})}(s_0 - (s'_2(x, y) - s_0)) = 2s_0 - s'_2(x, y).$$  

(19)

As a global algorithm, we construct the following optimization problem to calculate the solutions of the diffusion equations:

$$\tilde{s} = \arg\min_{s_2(x, y)} \int \int (u(x, y, \Delta t) - E_2(x, y))^2 dxdy. $$

(20)

However, the optimization process above is ill-posed [20], i.e., the minimum may not exist, and even if it exists, it may not be stable with respect to data noise. A common way to regularize this problem is to add a Tikhonov penalty

$$\tilde{s} = \arg\min_{s_2(x, y)} \int \int (u(x, y, \Delta t) - E_2(x, y))^2 dxdy + \alpha \|\nabla s_2(x, y)\|^2 + \alpha k \|s_2(x, y)\|^2$$

(21)

where the additional term imposes a smoothness constraint on the depth map. In practice, we use $\alpha > 0$, $k > 0$ which are all very small, because this term has no practical influence on the cost energy denoted as

$$F(s) = \int \int (u(x, y, \Delta t) - E_2(x, y))^2 dxdy + \alpha \|\nabla s\|^2 + \alpha k \|s\|^2.$$ 

(22)

Equation (23) is a dynamic optimization that can be solved by the gradient flow method. The algorithm can be divided into the following steps (the detailed process can be seen in [12]):

1) Give camera parameters $f, D, \gamma, v, s_0$; two defocus images $E_1, E_2$; a threshold $\epsilon$; $\alpha$ and optimization step $\beta$.
2) Initialize the depth map with a plan $s$; to be simple, we can suppose that the initial plane is an equifocal plane.
3) Compute (12), and get the relative blurring.
4) Compute (11), and get the solution $u(x, y, \Delta t)$ of the diffusion equations.
5) Compute (22) with the solution of step (4). If the cost energy is below $\epsilon$, the recurrence stops, or computes the following equation with step $\beta$:

$$\frac{\partial s}{\partial t} = -F'(s).$$

(24)

6) Compute (13), update the depth map, and return to step (3).

Therefore, if the initial depth is known, even if it is only an approximate value, the dynamic depth, as well as the expected shape, can be reconstructed.

IV. EXPERIMENT RESULTS

In order to validate the precision of the new algorithm, we tested it to reconstruct the bended shapes of a triangle cantilever and a conductive cantilever, respectively. In this experiment, we used the microscope HIROX-7700 shown in Fig. 6, and magnified the cantilevers 3500 times.

The rest of the parameters of the microscope are listed in the following: $f = 0.178$ mm, $s_0 = 3.4$ mm, $F$-number $= 2$, and $D = f/2$. The raise height of the cantilevers is controlled by Iphysik Instrumente (PI) nanoplatorm. First, we captured a defocused image of the cantilever. Then, the PI nanoplatorm, working up to the tip of the cantilever, rose to a desired height, and we
Fig. 7. Sketch of experiment setup.

Fig. 8. Two defocused images: (a) Left: image before depth variation; (b) Right: image after depth variation.

Fig. 9. Depth map of gray scale.

captured the other defocused image when the cantilever bended due to the press. The schematic illustration of the experiment is shown in Fig. 7. Furthermore, we provided the performance of the algorithm when the platform raised 500, 300, and 100 nm.

First, the experiment using the conductive cantilever was conducted. Fig. 8(a) shows the defocused image before depth variation and Fig. 8(b) shows the defocused image after depth variation; the computed depth map of grayscale is shown in Fig. 9; Fig. 10(a)–(c) shows the constructed 3-D shapes of the bended cantilever when the PI platform rises 500, 300, and 100 nm; the unit is in millimeter.

From Figs. 9 and 10, we can see that when the PI platform rises, the cantilever’s end with the tip bends obviously, and the deflection decreases gradually from this end to the other until it is close to a steady value; the bended degree is a monotonic function with the raise height. In order to validate the bended precision further, we give the cross section of the constructed shapes at the same position in Fig. 11. From it, we can see that the deflection height proportionately increases when the platform rises, and the height difference between the maximum value and the original value is exactly equal to the raise height of the PI platform.

Second, the experiment using the triangle cantilever was conducted. Fig. 12(a) shows the defocused image before depth variation and Fig. 12(b) shows the defocused image after depth variation; the computed depth map of grayscale is shown in Fig. 13; Fig. 14(a)–(c) shows the constructed 3-D shapes of the bended cantilever when the different raise height is 500, 300, and 100 nm; Fig. 15 shows the cross-sectional information. From them, we can get the same conclusion as the last experiment, but the reconstructed shapes are a little rough because the sensitivity of the triangle cantilever is lower.

From these experiments, we can see that, regardless of the cantilever shape, our algorithm can exactly reconstruct the
global bended shape with only two defocused images. The following conclusion can be given.

1) The most obvious bended field of a cantilever concentrates on the region near to the tip; it is reasonable because when the PI platform works up, all the stress concentrates on the tip due to our experiment theory.

2) The cantilever’s original shape, material, and illumination can influence the reconstruction results to some extent. For example, the conductive cantilever is thinner than the triangle cantilever, and the shape reconstruction of it is smoother due to its higher sensitivity; the black edge of the cantilever results in a little error in the result.

3) The raise height is larger, the calculation result is exacter, and the reconstruction image is smoother.

4) No matter how much the raise height is, the reconstruction height tends to be steady finally. Furthermore, the height difference between the maximum value and the original value is equal to the raise height of the PI platform.

V. CONCLUSION

In this paper, the global shape reconstruction of the bended AFM cantilevers is researched based on a global shape from defocus method. Our primary contribution is to suppose a new global SFD algorithm used to attain 3-D information in one-eye vision, hand-eye system, especially in micro/nanomanipulation. The second contribution is to perform the shape reconstruction experiments on different AFM cantilevers, and proposing a series of patterns on bended region, precision, and degree, which are absent in normal AFM imaging and force analysis. The results in the following are significant: computer vision can be used to reconstruct the global shape of samples in micro/nanomanipulation; our algorithm is an effective method to obtain the bended shape of the AFM cantilever. One of the most important contributions of this study is that it supplies a convenient method for research on further modeling cantilever bending and improving measurement accuracy of AFM.

There are several promising research directions for the future. Because the reconstruction result is sensitive to the cantilever’s shape, material, and illumination, a more stable and robust reconstruction method is needed. Also, based on the bended shape of the whole cantilever, we can calculate forces at each location of the cantilever and even construct the force model. From the real-time construction side, the calculation rate of our algorithm is needed to be studied.

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