Modeling and Simulation of an Atomic Force Microscopy System in the Z Direction

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Abstract. Atomic Force Microscopy (AFM) is a powerful tool in nanoscale imaging and manipulation. Many efforts have been made to improve its scanning rate by implementing many advanced controllers. The design of the controllers requires the achievement of the model of the AFM system, especially in the Z direction. The paper proposes a simple system identification method to estimate the model of the AFM in the Z direction by utilizing the experimental data. The simulation system is established to obtain the performance of controllers. Experiments demonstrate the simulation system is effective and helpful for the successful design and implementation of the controllers in the actual AFM system.

1. Introduction
The AFM is widely applied in many fields, such as chemistry, material science, biology and semiconductor industry [1]. It is used to trace the topography of specimens by a sharp tip supported on a micro cantilever. As the tip approaches to the sample, the cantilever gets deflected due to the tip-sample interaction. The deflection can be amplified by the optical lever system and then detected by the photo diode (PSD). The deflection can be compensated through the precisely controlled piezoelectric (PZT) scanner. An image is obtained by combining the lateral and the vertical positions of the scanner. The imaging rate is an important parameter for AFM. High-speed AFM could realize real time imaging in the above fields. However, the scanning rate is determined by the response rate of the feedback loop, which is seriously affected by the bandwidth of the scanner, the cantilever and the controller.

Recently, many research groups have proposed lots of schemes to realize high-speed AFMs [2-5], such as manufacturing smaller micro cantilevers [6, 7], designing highly rigid scanners [8, 9], implementing advanced controllers [10-16]. The utilization of smaller cantilevers and highly rigid scanners can increase the bandwidth of the system on the one hand, yet requires more complex crafts and increases the costs numerously on the other. By contrast, the design of the advanced controllers is simple and low-cost. Current commercial AFMs utilize simple PI controllers to control the precise motion of the PZT scanner. However, the high-order dynamics of the PZT can not be handled by the conventional PI controllers. Ando presents a dynamic PID controller to improve the robust of the feedback loop [10]. Schitter proposes a robust H∞ controller to realize the fast and precise position [13]. Osamah designs a robust adaptive controller to trace different specimens without modifying the gains [16]. The utilization of most advanced controllers requires modeling and simulating the system in the Z direction. However, most of the previously derived models involve complicated mathematical analysis, resulting in the realization of the advanced controllers being difficult.
To simplify the calculation process, the paper analyzes the AFM system in the Z direction and obtains a model of the system through a system identification scheme. Specifically, the Z feedback loop is considered as a black box model. The white noise signal as the input is utilized to drive the PZT scanner. The output of the PSD is recorded as the output signals. The model is estimated as a fixed order. By implementing the experimental inputs and outputs, the least square method is applied to identify the model. Then a robust adaptive controller is implemented through the model. By comparing with the conventional PI controller, the new advanced controller is verified to be more precise and robust.

2. System identification scheme
The AFM system in the Z direction is composed of a PZT scanner, a sample, a cantilever, a controller and a position sensitive detector (PSD). Each component needs to be analyzed to obtain the model. The piezoelectric scanner, resulting from its slow response characteristic, mainly reflects the mathematical model of the feedback system in the Z direction. The piezoelectric scanner is modeled as a single-input single-output system, as shown in Figure 1. A black box identification method is used in the experiment. The driving signal of the piezoelectric scanner and the PSD signal are considered as the input \( u(k) \) and the output \( y(k) \) of the black box respectively. A mica sample with very clean surface is used. The band-limited white noise signals \( e(k) \) with the frequency from 1kHz to 10kHz are generated as driving signals. The amplitude of the white noise signal is limited to 700mv to ensure that the system works in a linear state. First, the tip is tuned to contact the sample in closed-loop mode. Second, the feedback loop is turned off, and the acquisition card PXIe-6366 records the inputs and the outputs. Third, these data are analyzed using least square method to calculate the model in MATLAB.

![Figure 1. The experimental setup](image)

The calculation process is as follows. Figure 2 illustrates the mathematical model of the system. \( G(z^{-1}) \) presents the system model. The system noise is indicated by \( e(k) \). The input and the output are shown as \( u(k) \) and \( y(k) \), respectively.

![Figure 2. The model for system identification](image)

The discrete model of the AFM system can be described as Eq. 1.

\[
G(z^{-1}) = \frac{B(z^{-1})}{A(z^{-1})} = \frac{b_1 z^{-1} + b_2 z^{-2} + \ldots + b_n z^{-n}}{1 + a_1 z^{-1} + a_2 z^{-2} + \ldots + a_n z^{-n}}
\] (1)
Figure 2 can be expressed as Eq. 2.

\[ u(k) \cdot G(z^{-1}) + e(k) = y(k) \]  

(2)

Or

\[ y(k) \cdot A(z^{-1}) = u(k) \cdot B(z^{-1}) + e(k) \]  

(3)

u(k) is the piezoelectric scanner’s input voltage in the Z direction; y(k) is the photo diode measurement output; k is the discrete time; n is the order of the system; e(k) is the white noise signal.

The differential equation of Eq. 3 is as follows:

\[ y(k) = -a_1 y(k-1) - a_2 y(k-2) - \ldots - a_n y(k-n) + b_1 u(k-1) + b_2 u(k-2) + \ldots + b_n u(k-n) + e(k) \]

If

\[
\begin{bmatrix}
\phi(k) = [-y(k-1) & -y(k-2) & \ldots & -y(k-n) & u(k-1) & u(k-2) & \ldots & u(k-n)]^T \\
\theta = [a_1 & a_2 & \ldots & a_n & b_1 & b_2 & \ldots & b_n]^T
\end{bmatrix}
\]

Then Eq. 4 could be obtained.

\[ y(k) = \phi^T(k)\theta + e(k) \]  

(4)

If the number of the inputs and outputs is N respectively: \{ u(k), y(k) \}, k=1, 2, \ldots, n+N, then

\[ Y = \Phi \theta + e \]  

(5)

Y and e can be described as:

\[ Y = [y(n+1) \ y(n+2) \ \ldots \ y(n+N)]^T \]
\[ e = [e(n+1) \ e(n+2) \ \ldots \ e(n+N)]^T \]

So \Phi can be presented as:

\[
\Phi = \begin{bmatrix}
-y(n) & -y(n-1) & \ldots & -y(1) & u(n) & \ldots & u(1) \\
-y(n-1) & -y(n) & \ldots & -y(2) & u(n+1) & \ldots & u(2) \\
\vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
-y(n+N) & -y(n+N-1) & \ldots & -y(N) & u(n+N) & \ldots & u(N)
\end{bmatrix}
\]

J(\theta) can be defined as:

\[ J(\theta) = \sum_{i=1}^{N} (Y - \Phi \theta)^2 = \sum e^2(n+i) = e^T \cdot e = (Y - \Phi \theta)^T (Y - \Phi \theta) \]  

(6)

The least square method is to achieve the smallest J(\theta), so we can calculate its extreme value as Eq. 7.

\[ \frac{\partial J}{\partial \theta} = \frac{\partial}{\partial \theta} [(Y - \Phi \theta)^T (Y - \Phi \theta)] = 0 \]  

(7)

So the least square estimates of the system is shown in Eq. 8.

\[ \theta = (\Phi^T \Phi)^{-1} \Phi^T Y \]  

(8)

After sampling sufficient data, a sixth-order model (Eq. 9) of the feedback system can be obtained by employing the above least square method.
To prove that the model is accurate, a new set of data is input to the actual system and the above model respectively. Figure 3 illustrates a comparison between the simulated outputs of the identified model (solid curve) and the measured outputs of the system (dashed curve). The two curves fit well with each other showing only occasional separations. Figure 4 shows the bode diagram of the model, clearly illustrating that the first-order resonant frequency of the feedback loop is about 2.6 kHz.

\[
G(z) = \frac{-0.01017z^4 - 0.02301z^3 + 0.01025z^2 - 0.08255z - 0.2908}{z^5 - 0.89z^4 + 0.1435z^3 + 0.4535z^2 - 0.0189z - 0.1713} \quad (9)
\]

3. System identification scheme

To verify that the achieved model could be used to simulate the advanced controller, a robust adaptive controller is applied to compare with the conventional PI controller. The robust adaptive controller is designed according to the response rate of the system obtained from the above system identification scheme. It can tune the track parameters on basis of the topography and the scanning rate automatically. Specifically, the advanced controller could reserve enough time at the steps to wait for the response of the feedback loop. The square wave with 512 points is produced to simulate as a sample topography. The results are shown in Figure 5. The line image and the corresponding error signal achieved through the robust adaptive controller is shown in Figure 5 (a) (b). The line image and the corresponding error signal achieved through the robust adaptive controller is shown in Figure 5 (c) (d). Comparing Figure 5 (b) and Figure 5 (d), we can obtain that the advanced controller could adjust well at the steps. The experiments show that the model obtained through the system identification
method is effective. The modeling of the AFM system in the Z direction is helpful for the actual utilization of the advanced controller.

![Figure 5.](image)

**Figure 5.** The simulation results: (a) one line using constant rate scanning method; (b) control errors of one line using constant rate scanning method; (c) one line using the robust adaptive method; (d) control errors of one line using the robust adaptive method

4. **Conclusions**

The utilization of the advanced controller in AFM system requires the model of the AFM system in the Z direction. The paper proposes a simple system identification method to obtain the model. The model is proved suitable for the advanced controllers through simulations. The contrast experiments also verify that the advanced controller is more effective than the conventional PI controller. The future work will focus on the implementation of the new advanced controller in the actual AFM system.

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6. **References**

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