Virtual non-contact atomic force microscope

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Abstract. In this paper, the virtual atomic force microscope (AFM) is constructed on the basis
of the component models to simulate the conventional and high-speed AFMs. A room
temperature conventional AFM with its standard control system is used as a reference. The
virtual machine operates in non-contact mode (NC-AFM). The cantilever is oscillated at or
near its natural frequency with the amplitude of 1 nm to 100 nm above the sample. The tip-
sample interaction changes the amplitude, frequency, and phase of oscillation. In amplitude
modulated-AFM (AM-AFM), by measuring the tip vibration and extracting its amplitude, the
control system actuates the piezo-scanner to achieve the amplitude setpoint. By defining a
proper cost function, here settling time, optimum gain parameters for the control system are
obtained by the particle swarm optimization algorithm, PSO. Simulations are performed in two
steps: when only the Z-directional movement of the XYZ stage is considered and when raster
motion is considered. The performance of the new AFM is compared with a conventional AFM
via simulations.

Keywords: Virtual, AFM, Non-linear vibration, Non-contact mode, control system,
optimization algorithm, PSO.

Introduction

In the mid-1980s in order to magnify surface features in 3 dimensions the atomic force microscope
(AFM) [1], was developed. With the help of AFM, scanning of the object surface can be done up to
million times, which is extremely high magnifications. The other important feature of AFM is
scanning in three dimensions. Imaging of almost any type of surfaces can be done by AFM with an
atomic resolution [2].
Figure 1 Schematic basic AFM system

Figure 2 Schematic of cantilever interacting with the sample on the scanner

Schematic of a conventional AFM illustrated in Fig. 1 that consists of a microcantilever with a sharp tip, a piezo scanner, a photodetector, and control system [3-11].

Virtual AFM Modules

The virtual AM-AFM is constructed in the modular form using MATLAB functions to study the performance of the high-speed AFM. The individual AFM component models are integrated into a control loop to perform scanning simulations. The main module of the virtual AFM simulates the cantilever interacting with the sample placed on the piezo-scanner, which is schematically shown in Fig. 2. In addition, the variables used in the control loop are defined in Fig. 3.

Figure 3 Virtual non-contact AFM modules

The complete model of the scanning system shown in Fig. 3 includes the following modules:
1. Sample topographic simulator,
2. System dynamics,
3. Amplitude calculation,
4. PI controller,
5. Z motion of the XYZ stage,
6. X motion of the XYZ stage.

These modules are discussed in the following subsections.
**Sample Topographic Simulator**

This function simulates sample topographic features in a scan line. In fact, the sample topography involves many scan lines with different topographic information. The shape of the scan line could be sinusoid, toothed, or other forms. Here, we use a silicon wafer with SiO2 layer calibration and test specimen (629-30, Ted Pella, Inc.) illustrated in Fig. 4 (left) as a reference for the sample topographic simulator. However, in simulations, it is quite adequate to utilize one scan line (Fig. 4 (right)).

**Figure 4** Silicon wafer with SiO2 layer calibration and test specimen. Perspective view (right), A scan line in the X-Z plane (left)

**System Dynamics**

In this paper, the lumped parameter model has been used. The lumped parameter model of the cantilever consists of an effective mass \( m_e \) at the end of a massless spring with the stiffness of \( K \) as illustrated in Fig. 2.

Cantilever excited by an external driving force \( F_{EXT} = F_0 \cos(\Omega t) \), and \( P(Z(t)) \) is the force acting on the tip resulting from the tip-sample interaction. For non-contact AFM, van der Waals sphere–plane interaction is used as \([13, 4]\) \( P(Z(t)) = -A_H R / 6(Z_0 - Z)^2 \), where \( A_H, R \) and \( Z_0 \) are the Hamaker constant, the tip apex radius, and the distance from the fixed base frame coordinate to the sample, respectively.

The dimensionless equation of motion is obtained as \([12]\):

\[
\frac{d^2x}{d\tau^2} + b \frac{dx}{d\tau} + x = p \cos((1 + \varepsilon \sigma)\tau) + \frac{d}{(\eta - x)^2},
\]

\( \Omega = \omega_0 + \varepsilon \sigma, \)

where \( \varepsilon \) is a small parameter and \( \sigma \) is a detuning parameter which describes the nearness of \( \Omega \) to \( \omega_0 \), the fundamental resonance frequency of the cantilever.

**Amplitude Calculation**

This function takes the tip deflection signal as an input and computes the amplitude of oscillation using a peak-to-peak amplitude calculation method. The steady state of oscillation is estimated and a half of the difference between the minimum of local minimum points and maximum of local maximum points in one period is taken as the amplitude.

**PI Controller**

AM-AFM requires a control loop to keep the cantilever vibration amplitude at a preset value \( A_{set} \). For this purpose, a PI controller is used to control the vertical movements of the XYZ stage. It has an analog to digital converter that samples the error signal at a fixed sampling rate. A built-in block is
utilized to actuate the XYZ stage based on the error in the peak-to-peak amplitude of the cantilever oscillations ($A_{set} - A$).

In order to find optimum gain values for the PI controller, the particle swarm optimization algorithm, PSO, is used [13]. By defining a proper cost function, here settling time, optimum gain parameters are obtained by PSO.

Fig. 5 shows the step response of the XYZ stage for randomly selected and optimum gain parameters. The optimum gain parameters obtained by the PSO algorithm are $K_p=1$ and $K_i=0.005$. The step response of the XYZ stage for optimum gain parameters is about two times faster than the response for the other gain parameters as shown in Figs. 5.

![Figure 5](image)

**Figure 5** Step response of the XYZ stage for various gain parameters (left) and optimum gain parameters (right). $K_p=1$ in both diagrams

**Z Motion of the XYZ Stage**

The schematic diagram of the second order model is shown in Fig. 6. The variables $x_1$ and $x_2$ denote the positions of the center of the masses. The mass $m_1$ represents the upper half of the Z-piezo plus the mass of the sample. The lower half of the Z-piezo lumped with the effective mass of the supporting structure is marked as $m_2$, which has the effective spring constant $k_2$, and the effective damping coefficient $c_2$. It is assumed that the force $F$ is exerted between the masses $m_1$ and $m_2$ by the piezo. The elongation of the piezo stack is obtained from $L = x_1 - x_2$.

It should be noted that the elongation of the piezo stack is considered as the input when its dynamics are neglected. The transfer function from $L$ to $x_1$ is:

$$G_{Z,L}(s) = \frac{m_2 s^2 + c_2 s + k}{(m_1 + m_2) s^2 + c_2 s + k}.$$  (2)

For vertical movements of the XYZ stage, the transfer function obtained in Eq. 2 for the scanner in the Z-direction is used to build the virtual AFM. The output of the XYZ stage function is the position of the surface of the XYZ stage relative to its base, i.e. $Z_{in}$. As mentioned before, the PI controller adjusts the vertical movements of the XYZ stage.
X Motion of the XYZ Stage

In order to perform line-scanning simulations, X-directional movements of the stage should be modeled. In this study, the lumped parameter model used for modeling of the mechanical scanner (Fig. 7).

The raster motion of the scanner system is modeled by three masses supported by spring between them. \( m_3 \) is the mass of the main moving body, and \( m_1 \) and \( m_2 \) are the mass of the intermediate body lumped with the effective mass of the supporting structure, which has the effective spring constant \( k \). \( F_p \) is an external force which is produced by the piezo-actuator. By using the notation in Fig. 7, one can write the transfer function the transfer function between \( x_3 \) and \( F_p \) that is:

\[
G(s) = \frac{X_3(s)}{F_p(s)} = \frac{m_3 s^2 + 2k}{m_1 m_3 s^4 + 2k(m_1 + m_3) s^2 + 2k^2}.
\]  

(3)

Dynamics of the piezoelectric actuator is neglected because its dynamics is very fast compared to that of the stage. Therefore, we can model it only as a force generating capacitance element as shown in Fig. 8. Based on this assumption, the induced force and applied voltage are related by

\[
F_p = F_{cf} V_o.
\]  

(4)

![Figure 8 Piezoelectric actuator model](image)

where \( F_{cf} \) is a constant related to the geometry and physical properties of the piezo-material, and \( V_o \) is the voltage applied to the electrodes.

Taking the Laplace transforms, the transfer function is obtained as in \( s \) domain:

\[
G_c(s) = \frac{V_o(s)}{V_i(s)} = \frac{1}{RC s + 1}.
\]  

(5)

In addition to the X-directional stage model presented in Eq. 3, the control loop of the X-directional motion shown in Fig. 9 includes the following components:

A. Driving circuit
The driving circuit model presented in Eq. 5 is used for this function. Its input is control signal from the PID controller and its output is the voltage applied on the piezo-actuator.

B. Piezo-actuator
The piezo-actuator is modeled as a force generating capacitance element described in Eq. 4. The PID controller adjusts the force generated by the piezo-actuator.

C. PID controller
This module is used to control X-directional movements of the stage. A built-in block is utilized to actuate the X-directional stage based on the error signal \((x_{3d} - x_3)\). In order to find optimum gain values for the PID controller, the PSO algorithm is used. By defining a proper cost function, here settling time, optimum gain parameters are obtained by PSO.

![Figure 9](image)

**Figure 9** The control loop of x-directional motion

![Figure 10](image)

**Figure 10** Step response of x-stage for optimum gain parameters

Figs. 7 (left) and (right) show the effect of the gain parameter \(K_p\) and \(K_d\) on the step response of the x-stage while the other gain parameters are kept constant, respectively.

The optimum gain parameters obtained by the PSO algorithm are \(K_p = 3000\), \(K_i = 50000\), and \(K_d = 1000\). The step response of the x-stage for optimum gain parameters is about three times faster than the response for the other gain parameters as shown in Fig. 10.

**Results**

Simulations are performed in two steps:

1. When the only the Z-directional movement of the XYZ stage is considered.
2. When raster motion is also considered.

In simulations, the resonance frequency of the scanner is assumed to be 35 KHz, obtained for the high-speed AFM and 10 KHz for the conventional AFM.

The first simulation is carried out by utilizing one scan line and considering only the vertical motion of the XYZ stage. The sample generated by the topographic simulator shown in Fig. 4 (right) is used in the simulation. The input, output, and error of the output with respect to the input are shown in
Fig. 11. The elapsed time to obtain the output is 2.484 seconds for the high-speed AFM and 3.742 seconds for the conventional AFM. In this simulation, the number of points which was probed by the tip, i.e. the number of pixels in one scan line is 132.

In the previous simulations, only the vertical motion of the XYZ stage has been considered. Now, the X-directional motion of the stage is taken into account by using three different raster speeds. The sample generated by the topographic simulator shown in Fig. 4 (bottom) is used in the simulation. The input, output, and error of the output with respect to the input are shown in Figs. 12-13. The elapsed time to obtain the output and the corresponding number of pixels are shown in Table 1.

![Figure 11](image1.png)

**Figure 11**  Simulation of high-speed virtual AFM (elapsed time: 2.4845 seconds, pixels: 132)

![Figure 12](image2.png)

**Figure 12**  Simulation of high-speed virtual AFM (elapsed time: 21.38 seconds, pixels: 1300)

![Figure 13](image3.png)

**Figure 13**  Simulation of high-speed virtual AFM (elapsed time: 6.459 seconds, pixels: 132)
Table 1. Simulation times of high-speed virtual AFM for various raster speeds

| Raster speed | Simulation time (seconds) | Number of pixels |
|--------------|---------------------------|------------------|
|              | High-speed AFM            | Conventional AFM |
| 16 nm/s      | 21.380 sec.               | 32.070 sec.      | 1300 |
| 160 nm/s     | 6.459 sec.                | 9.646 sec.       | 132  |
| 1.28 μm/s    | 0.739 sec.                | 1.108 sec.       | 14   |

Conclusion

In this paper, the virtual atomic force microscope (AFM) is constructed on the basis of the component models to simulate the conventional and high-speed AFMs. A room temperature conventional AFM with its standard control system is used as a reference. The virtual machine operates in non-contact mode (NC-AFM). The cantilever is oscillated at or near its natural frequency with the amplitude of 1 nm to 100 nm above the sample. The tip-sample interaction changes the amplitude, frequency, and phase of oscillation. In amplitude modulated-AFM (AM-AFM), by measuring the tip vibration and extracting its amplitude, the control system actuates the piezo-scanner to achieve the amplitude setpoint. Simulations are performed in two steps: when only the Z-directional movement of the XYZ stage is considered and when raster motion is considered.

According to the simulation results, it can be concluded that the scanning speed of the high-speed AFM is 1.5 times of the conventional AFM.

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