Influence of a Heterogeneous Sample Surface on a Driven Microcantilever Probe Model

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Abstract

An atomic force microscope (AFM) is a microscope that measures the information of a sample surface when the probe tip approaches the surface. In our previous work, we investigated a mass-spring model of the driven probe tip influenced by a homogeneous sample. In this study, we investigate the influence of a heterogeneous sample surface on the amplitude characteristic of the tip oscillation by comparing the calculated amplitude and the theoretically obtained amplitude using a bifurcation theory.

1. Introduction

A scanning probe microscope (SPM) is a microscope that measures the information of a sample surface when the probe tip approaches the surface. Owing to the necessity of obtaining the information of microscopic samples, such as nanoscale semiconductor devices, studies on the mechanical behavior of the probe tip have attracted considerable research interests [1–6]. Dynamic atomic force microscope (dAFM) is one type of SPM. An external harmonic force is injected into the probe, which is set at an equilibrium distance from the sample surface. The sample information is obtained by detecting the amplitude or frequency modulations of the tip oscillation originating from the interaction force between the tip and the sample.

In our previous work, we investigated a mass-spring model of the driven probe tip influenced by a homogeneous sample [6]. In this study, we investigate the influence of a heterogeneous sample surface on the amplitude characteristic of the tip oscillation. The heterogeneous sample consists of five distinctive regions where the equilibrium distances from the sample are set to be different from each other. By changing the scanning point in the x–y plane, we calculate the amplitude of oscillation in the steady-state. Assuming a heterogeneous sample surface, we investigate how the interaction force affects the tip oscillation using a color map. In addition, by comparing the calculated amplitude and the theoretically obtained amplitude using a bifurcation theory, we investigate the variation of the mean square error as a function of the intensity of the external force.

2. Driven Microcantilever Probe Model

In this study, we approximate the driven lateral oscillation of the probe tip by using a simple mass-spring model, which consists of an effective mass \( m \) [kg] and a spring with a spring constant \( k \) [kg/s^2]. When the probe tip is driven by an external force \( l \cos(\omega t) \) [m] at a distance \( z_0 \) [m] from the sample surface, the lateral oscillation \( z' \) [m], which is shown in Fig. 1, is written as follows [6]:

\[
m \frac{d^2 z'}{dt^2} + \frac{m \omega_0^2}{Q} \frac{dz'}{dt} + m \omega_0^2 (z' - z_0) = ml \omega_0^2 \cos(\omega t) + F(z')
\]

where the variable \( t \) [s] corresponds to the time variable. The parameters \( Q(= m \omega_0^2/C) \) and \( \omega_0(\sqrt{k/m}) \) [rad/s] represent the quality factor (fixed as \( Q = 100 \) in this study) and the natural frequency of the probe, respectively. Furthermore, \( F(z') \) [N] corresponds to the nonlinear interaction force, which is divided into the attractive and repulsive regions in terms of the tip sample distance, derived from the Lenard-Jones potential, which is given as follows:

\[
F(z') = 8R_0\pi^2 \varepsilon_L \rho_0^2 \sigma^2 \left\{ \frac{1}{5} \left( \frac{z}{\sigma} \right)^{10} - \frac{1}{2} \left( \frac{z}{\sigma} \right)^{11} \right\} + 8\pi \varepsilon_L \rho_0 \sigma \left\{ \left( \frac{z}{\sigma} \right)^{11} - \left( \frac{z}{\sigma} \right)^5 \right\}
\]

Figure 1: Mass spring model
where, \( R_0 \) [m], \( \varepsilon_{LJ} \) [J], \( n_0 \) [m\(^{-2}\)], and \( \sigma \) [m] represent the probe radius of curvature, the cohesion energy of a neutral atom, the number of atoms per unit area, and the distance between atoms in equilibrium, respectively. In this study, we assume that both the probe tip and the sample surface are composed of silicon, which fix the physical parameters as \( \varepsilon_{LJ} = 1.602 \times 10^{-21} \) [J], \( n_0 = 1.11 \times 10^{19} \) [m\(^{-2}\)], and \( \sigma = 0.25 \times 10^{-9} \) [m]. In addition, we also set \( m = 5.17 \times 10^{-12} \) [kg], \( R_0 = 15 \times 10^{-9} \) [m], and \( \omega_0 = 2\pi \times 70 \times 10^3 \) [rad/s] referring to the specifications of the actual microcantilever probe OMCL-AC240TM [7].

\[
\begin{align*}
\varepsilon &= \frac{z_0}{\sigma}, \quad a_e = \frac{l}{\sigma}, \quad \omega_1 = \frac{\omega}{\omega_0}, \quad \tau = t\omega_0, \quad z = \frac{z'}{\sigma}, \\
\mu_1 &= \frac{8}{m\omega_0^2} R_0 \pi^2 \varepsilon_{LJ} n_0^2 \sigma, \quad \mu_2 = \frac{8}{m\omega_0^2} \pi \varepsilon_{LJ} n_0 \sigma
\end{align*}
\]

By substituting the following variables and parameters into Eq. (1),

\[
\begin{align*}
\varepsilon &= \frac{z_0}{\sigma}, \quad a_e = \frac{l}{\sigma}, \quad \omega_1 = \frac{\omega}{\omega_0}, \quad \tau = t\omega_0, \quad z = \frac{z'}{\sigma}, \\
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\end{align*}
\]

the normalized version of equation of motion is written as follows:

\[
\frac{d^2z}{d\tau^2} + \frac{1}{Q} \frac{dz}{d\tau} + (z - \varepsilon) = a_e \cos(\omega_1 \tau) + F(z)
\]

where the normalized interaction force is given by

\[
F(z) = \mu_1 \left\{ \frac{1}{5} z^{-10} - \frac{1}{2} z^{-4} \right\} + \mu_2 \left\{ z^{-11} - z^{-5} \right\}
\]

In the following results, the frequency of the external force is set to the natural frequency of the probe \((\omega_1 = 1.0)\). Figure 2 shows the normalized interaction force as a function of \( z \), where the parameters are fixed as \( \mu_1 = 58.436 \) and \( \mu_2 = 0.4469 \) in this study.

We investigate the influence of the heterogeneous sample surface as shown in Fig. 3, where the heterogenous sample consists of five distinctive regions \((\varepsilon = 12, 14, 16, 18, \text{ and } 20)\). Then, we use the calculated data for \( \tau \geq 1,000 \) to ignore the transient state. By changing the scanning point from the left bottom to the upper right, discretized with a step size of \((\Delta x = \Delta y = 1)\) in the \(x-y\) plane, we calculate the amplitude of oscillation in the steady-state. We numerically calculate Eq. (4) when the quality factor is set to \( Q = 100 \) by using the fourth order Runge-Kutta method with a step size of \(2\pi/(8192\omega_1)\).

By substituting the following variables and parameters into Eq. (1),

\[
\begin{align*}
\varepsilon &= \frac{z_0}{\sigma}, \quad a_e = \frac{l}{\sigma}, \quad \omega_1 = \frac{\omega}{\omega_0}, \quad \tau = t\omega_0, \quad z = \frac{z'}{\sigma}, \\
\mu_1 &= \frac{8}{m\omega_0^2} R_0 \pi^2 \varepsilon_{LJ} n_0^2 \sigma, \quad \mu_2 = \frac{8}{m\omega_0^2} \pi \varepsilon_{LJ} n_0 \sigma
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\frac{d^2z}{d\tau^2} + \frac{1}{Q} \frac{dz}{d\tau} + (z - \varepsilon) = a_e \cos(\omega_1 \tau) + F(z)
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3. Results

It is known that the tip-oscillation has two coexisting solutions when the distance between the tip and sample becomes small [6]. One is a solution in which the tip does not contact with the sample, while the other is a solution in which the tip
on the sample is assumed. That is, the influence of the basin surface in Fig. 3 on the steady-state amplitude in terms of a parameter set is investigated. To realize this condition, the initial condition of the probe tip at each scanned point on the sample is set by using a continuous deformation method, where the value of the final state at the previous scanned point is applied to the present initial condition. Figure 5 (a) shows the numerically obtained peak-to-peak amplitude of oscillation when the amplitude of external force \( a_e \) is set to 0.12, where a brighter color indicates a larger amplitude of the tip-oscillation. For \( a_e = 0.12 \), because the external force is weakly injected into the probe, it is difficult to distinguish the heterogeneous sample surface. In contrast, for larger \( a_e = 0.2 \), the sample surface is successfully measured as shown in Fig. 5 (b). Moreover, Fig. 5 (c) shows the peak-to-peak amplitude of oscillation for \( a_e = 0.36 \). The region filled with the brightest red color, which appears for \( \varepsilon = 0.20 \) and 0.18, corresponds to the part where a large amplitude of oscillation appears. Therefore, it is expected that there exists an appropriate intensity of the external force in AM-AFM.

To investigate the influence of the value of \( a_e \) further in detail, we investigate quantitatively the mean square error between the calculated peak-to-peak amplitude and the theoretically obtained amplitude \( = \langle E \rangle \). The theoretical value is obtained by the following procedure. First, we precisely obtain the stable fixed point of the small amplitude of oscillation by using the shooting algorithm [8]. Next, by applying the fixed point to the initial condition in Eq. (4), the value of the peak-to-peak amplitude of the small amplitude oscillation \( z_{pp}(\varepsilon, a_e) \) is calculated. We calculate the five distinctive values \( z_{pp}(\varepsilon, a_e) \) for \( \varepsilon = 12, 14, 16, 18, \) and 20 as a function of \( a_e \).

Because the initial condition is precisely put on the attractor of the small amplitude of oscillation, the obtained value of \( z_{pp}(\varepsilon, a_e) \) can be regarded as the approximated theoretical value of the small amplitude of oscillation for the fixed value of \( \varepsilon \). Then, we calculate the mean square error of all the scanned points (the number of points is \( 20 \times 20 = 400 \)) between \( z_{pp} \) and \( z_{pp}(\varepsilon, a_e) \) for the fixed values of \( \varepsilon \) and \( a_e \).

Figure 6 shows the mean square error of all the scanned points in Fig. 3 as a function of \( a_e \). It is shown that the first zero of the mean square error occurs at \( a_e = 0.162 \). Therefore, for this value of \( a_e \), it is confirmed that the sample surface is successfully measured. In contrast, for \( a_e > 0.283 \), the mean square error increases significantly, because the steady-state solution changes from the small amplitude solution into the large amplitude solution due to the relatively large amplitude of oscillation of the external force. For \( 0.162 \leq a_e \leq 0.282 \), the value of the mean square error shows a damping oscillation as a function of \( a_e \). Figure 7 shows the mean square errors of the scanned points in the five distinctive regions in Fig. 3 as a function of \( a_e \).

1We regard the point where \( < E > \) becomes smaller than \( 7.0 \times 10^{-6} \) the zero point due to the precision of the step size of the time variable in the numerical integration.
this figure, qualitatively same results are calculated for all the values of $\varepsilon$ except for the values of the first zero.

**Figure 6:** Mean square error of all the scanned points in Fig. 3 as a function of $a_e$

4. Conclusions

This study investigated the influence of a heterogeneous sample surface on the amplitude characteristic of the probe tip in a micro-cantilever probe model for AFM with one degree of freedom. By investigating the steady-state amplitude of the probe oscillation, it was verified that there is an appropriate value of amplitude for the external oscillation. In addition, we calculated the mean square error of the scanned points as a function of $a_e$ by comparing the numerically calculated peak-to-peak amplitude with the theoretically obtained amplitude. The origin of the damping oscillatory phenomenon observed in a certain parameter region of $a_e$ remains to be investigated in our future work.

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**References**


