

Numerical simulation of nano scanning in intermittent-contact mode AFM under Q control

A Varol, I Gunev, B Orun and C Basdogan¹

College of Engineering, Koc University, Istanbul, 34450, Turkey

E-mail: cbasdogan@ku.edu.tr

Received 20 September 2007, in final form 30 November 2007

Published 29 January 2008

Online at stacks.iop.org/Nano/19/075503

Abstract

We investigate nano scanning in tapping mode atomic force microscopy (AFM) under quality (Q) control via numerical simulations performed in SIMULINK. We focus on the simulation of the whole scan process rather than the simulation of cantilever dynamics and the force interactions between the probe tip and the surface alone, as in most of the earlier numerical studies. This enables us to quantify the scan performance under Q control for different scan settings. Using the numerical simulations, we first investigate the effect of the elastic modulus of the sample (relative to the substrate surface) and probe stiffness on the scan results. Our numerical simulations show that scanning in an attractive regime using soft cantilevers with high effective Q factor (Q_{eff}) results in a better image quality. We then demonstrate the trade-off in setting Q_{eff} of the probe in Q control: low values of Q_{eff} cause an increase in tapping forces while higher ones limit the maximum achievable scan speed due to the slow response of the cantilever to the rapid changes in surface profile. Finally, we show that it is possible to achieve higher scan speeds without causing an increase in the tapping forces using adaptive Q control (AQC), in which the Q factor of the probe is changed instantaneously depending on the magnitude of the error signal in oscillation amplitude. The scan performance of AQC is quantitatively compared to that of standard Q control using iso-error curves obtained from numerical simulations first and then the results are validated through scan experiments performed using a physical set-up.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

In tapping mode dynamic force microscopy (DFM), a cantilever probe, oscillating in free-air around the resonant frequency with an amplitude of A_0 , is used to scan a sample surface [1]. When the tip of the probe taps the sample surface lightly for a very short period of time, the oscillation amplitude is reduced to $A < A_0$. In an amplitude modulation scheme, a scan controller moves the sample or the probe along the vertical direction (i.e. the z -direction) such that the oscillation amplitude during tapping stays constant at a set amplitude, A_{set} . These up and down movements along the vertical direction are recorded during scanning to construct the surface profile of the sample.

During tapping mode scanning, the interaction forces between the probe tip and the sample surface are highly nonlinear and the response of the cantilever probe to these forces is primarily governed by its quality factor, $Q = \Delta\omega/\omega_r$, where ω_r is the resonance frequency of the cantilever and $\Delta\omega$ is the width of the resonance curve for which the energy is at least half of its peak value at the resonance frequency. The Q factor of a cantilever probe indicates its energy dissipation capacity and the damping present in the system. A probe with a low Q factor dumps its energy faster, resulting in lower-amplitude steady-state oscillations and a rounded resonance curve. On the other hand, a probe with a high Q factor oscillates at higher amplitudes around the resonance frequency and its resonance curve has a sharp peak.

The Q factor of a cantilever probe can be adjusted using a feedback circuit. By applying an appropriate force to the

¹ Author to whom any correspondence should be addressed.

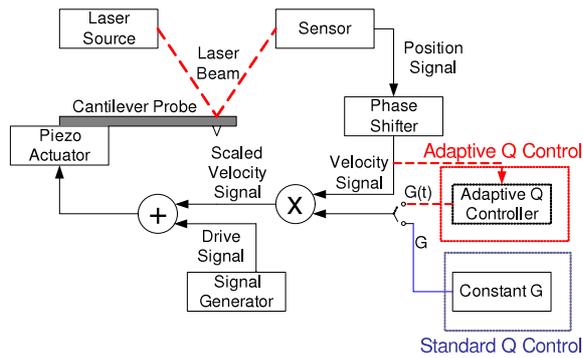


Figure 1. A schematic representation of a driven cantilever probe in tapping mode scanning under standard (blue solid line) and adaptive (red dashed line) Q control. The gain G is constant in standard Q control whereas it is adjusted in real time based on the surface profile in adaptive Q control.

oscillating cantilever, its motion can be regulated in such a way that the modified response of the system shows an increased or decreased Q factor. This approach is known as ‘ Q control’ and has been suggested as an effective scanning method in DFM [2]. In figure 1, a schematic illustration of a Q controlled cantilever probe is presented. Typically, a phase shifter and an amplifier with a gain G are used in the feedback circuit in order to control the Q factor of an oscillating cantilever. First, the displacement signal of an oscillating probe is measured using a photo-detector, shifted in phase using the phase shifter, and then scaled by the gain G , and finally used as the velocity signal in the feedback loop. This velocity signal is added (or subtracted from) the driving signal to decrease (or to increase) the effective damping of the cantilever. In the text, we hereafter will call this approach where the gain G is set to a constant value before the scan process as standard Q control.

Former studies have shown that the image resolution improves with Q control, but the mechanism for this is not well understood [3–5]. Rodriguez and Garcia developed an analytical solution for an oscillating probe under Q control [6]. Their simulations suggested that the slope of the amplitude–distance curves is substantially larger, implying a higher sensitivity to tip–surface variations, which results in better image quality. However, numerical simulations performed later by Kokavecz *et al* yielded that the slope of the amplitude versus distance curves is not increased for stiff samples and hence they concluded that the maximal probe sensitivity cannot be increased with Q control [7]. Holscher *et al* performed numerical simulations and showed that an increased Q factor prevents the oscillating cantilever from jumping into a repulsive imaging regime during tip–sample approach, which often occurs in tapping mode scanning without Q control [8]. They concluded that restriction of the maximal tip–sample force to specific parts of the attractive regime in Q control is the main reason for the enhanced imaging quality. Hence, it can be argued that Q control keeps the probe in the attractive regime longer, and as a result the magnitude of the average tapping forces is reduced. In fact, Jäggi *et al* experimentally determined that the average tip–sample forces are reduced by Q control [9].

On the other hand, there is a trade-off between tapping forces and scan speed when setting the Q factor of a scanning probe, which has not been investigated in detail. For example, when scanning in liquid, the Q factor of the probe is increased to obtain better scan results and prevent damage on the sample [10]. However, the mechanical sensing bandwidth of the probe is inversely proportional to its Q factor, and increasing it limits the maximum achievable scan speed (i.e. the maximum speed at which the probe can trace the sample surface with a reasonable amount of positional error in the scan profile). Sulchek *et al* showed that the sensing bandwidth of a scanning probe and scan speed can be improved significantly by actively lowering the Q factor of the probe when scanning nano surfaces in air [11, 12].

In standard Q control, achieving higher scan speeds with reduced tapping forces is not possible since the effective Q factor (Q_{eff}) of the probe is set to a value that is lower or higher than its native one before scanning. Gunev *et al* suggested that these two benefits can be realized simultaneously using adaptive Q control (AQC) [13]. They developed a signal processing circuit that adjusts the gain G on the fly during scanning depending on the error in amplitude signal. If there is a tendency towards saturation in error (as typically occurs in scanning steep downward steps), the controller increases the Q factor of the probe rapidly to avoid the problem.

In this study, we investigate nano scanning in tapping mode atomic force microscopy (AFM) under Q control via numerical simulations. We first explore the influence of the elastic modulus of the sample material (relative to the substrate surface) and probe stiffness on scan performance. We then show the trade-off between scan speed and tapping forces in setting the Q factor of the probe. Finally, we demonstrate that AQC solves the trade-off problem and expands the allowable workspace of the scan controller. In most of the earlier studies involving numerical simulations, only the cantilever dynamics has been investigated, but the transient effects during scanning have been neglected (i.e. only the steady-state solution of cantilever oscillations is considered). These studies have primarily investigated the effect of various parameters and tip–sample forces on the cantilever dynamics. Moreover, the parameters of the cantilever model used in these simulations are not obtained from the experimental measurements and are mostly selected somehow arbitrarily to meet the simulation needs. We categorize these types of numerical studies as ‘cantilever’ simulations to differentiate them from our work on ‘scanning’ simulations. To our knowledge, there are only a few studies focusing on the end-to-end simulation of the whole scan process [14]. Our simulations not only integrate the model of a cantilever but also the models of other components of a typical AFM system such as the scan controller, measurement devices and a DAQ sampling unit. This is achieved using SIMULINK, which provides a flexible computing environment for supporting linear and nonlinear systems, modeled in continuous time, sampled time or a hybrid of the two. The detailed models of the components used in our simulations are discussed in the upcoming sections.

2. Set-up

Our numerical simulations are supported by the experiments conducted using a home-made AFM set-up. The major components of our AFM set-up include a self-actuated AFM probe which is brought close to a sample surface using an XYZ manual stage, a computer controlled XYZ nano stage for moving the sample surface with respect to the probe, and a laser Doppler vibrometer (LDV) for measuring the vertical vibrations of the probe. An analog signal processing circuit consisting of (a) a root mean square (RMS) converter, (b) a variable phase shifter and (c) a voltage multiplier is built and integrated into the AFM set-up to adaptively modify the Q factor of the probe on the fly during scanning. Details about the set-up and the components are available in our earlier publication [13].

In order to scan a sample using the developed AFM system, the velocity of the probe tip is measured as a continuous signal using the LDV and then the RMS value of this signal is calculated over a running window and sampled by a DAQ card into a computer. The oscillation amplitude of the probe A is calculated from the RMS signal and then compared with the desired oscillation amplitude A_{set} . A proportional integral (PI) controller developed in LabVIEW keeps the vibration amplitude of the probe constant during raster scanning by moving the nano stage up and down along the Z-axis based on the error signal ($A_{set} - A$).

3. Cantilever dynamics

3.1. Cantilever model

A damped mass-spring system is used to model the dynamical behavior of the cantilever. This model is a reasonable approximation of the oscillating cantilever and frequently utilized in earlier AFM studies [10, 15, 16]. It is assumed that the cantilever is externally driven by a sinusoidal force F_{drive} at its resonance frequency. In addition to the driving force, the oscillations of the cantilever are also influenced by the interaction forces between the cantilever tip and sample surface, F_{ts} . This force is a function of the tip-sample separation distance, h . The dynamics of the cantilever probe can be written as a second-order differential equation in the form of

$$m\ddot{z} + b\dot{z} + kz = F_{drive} + F_{ts}(h) \quad (1)$$

where k and m are the effective spring constant and mass of the cantilever, respectively. In addition, a damper with a coefficient b is added to the model to simulate damping due to air. The damper applies a resistance to the oscillations proportional to the vibration velocity of the cantilever and causes energy dissipation. Expressing the above equation in terms of measurable quantities, we have the following equation:

$$m\ddot{z} + \frac{m\omega}{Q}\dot{z} + kz = F_0 \cos(\omega t) + F_{ts}(h) \quad (2)$$

where ω and F_0 are the frequency and the magnitude of the external driving force, respectively (the cantilever probe

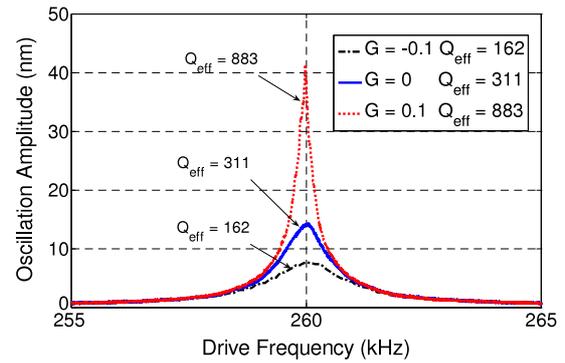


Figure 2. The amplitude response of the cantilever around the resonance frequency for different values of effective quality factor is obtained through experimental measurements.

is actuated at its resonance frequency, $\omega = \omega_r$). The Q factor of the cantilever is inversely proportional to the damping coefficient b . For a system with a high Q factor (low damping), the resonance frequency of the system is approximately equal to its natural frequency, $\omega_r \approx \omega_n = \sqrt{k/m}$. The Q factor and the resonance frequency of the cantilever can be determined experimentally by examining its frequency response. The frequency response of the cantilever used in our experimental set-up and numerical simulations is plotted for different gains G (figure 2). From the plots, the resonance frequency of the cantilever (260 kHz) is determined as the frequency at which the oscillation amplitude reaches a maximum and the Q factor of the probe ($Q_{native} = 311$) is determined by measuring the frequency range $\Delta\omega$ where the energy of the oscillations is at least half of the maximum energy at the resonance frequency. The value of the spring constant used in the numerical model is obtained from the cantilever manufacturer's catalog (the nominal value is reported as 3 N m^{-1} at the operating frequency).

3.2. Force interactions

The force interaction between the probe tip and sample geometry is modeled as a spherical object interacting with a flat surface [17–19]. In the tapping mode AFM, the cantilever is oscillated over the sample surface and contacts the surface for a brief period of time at each oscillation cycle. As a result, the distance h between the cantilever tip and sample surface changes continuously (figure 3(a)). Depending on the separation distance, two different interaction models are typically utilized to calculate the tip-sample forces.

- (1) *Non-contact forces*: For separation distances larger than the inter-atomic distance a_0 , the long-range attractive force is dominant (note that electrostatic interactions are ignored). The attraction results from the integration of van der Waals energy between two atoms over the atoms of interacting surfaces. The van der Waals attraction force between a sphere and a flat surface is the negative gradient of this energy and can be written as a function of tip-sample separation distance h , the tip radius R and the

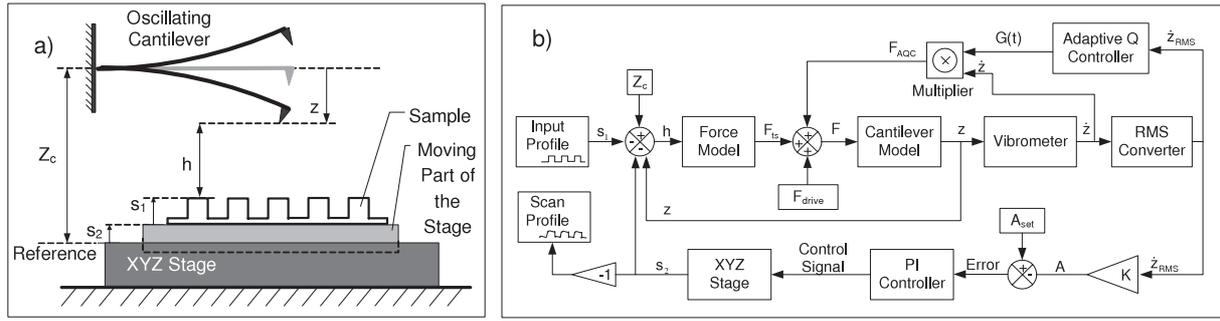


Figure 3. SIMULINK model of our experimental scanning set-up.

Hamaker constant H as follows [20]:

$$F_{vdw}(h) = -\frac{HR}{6h^2} \quad \text{if } h > a_0. \quad (3)$$

- (2) *Contact forces*: It is assumed that a mechanical contact between the cantilever tip and the sample surface occurs when the separation distance h is smaller than the inter-atomic distance a_0 (negative values of h indicate indentation into the sample surface). During the contact, both adhesive and repulsive forces are effective. According to the DMT theory [21], the adhesion force is equal to the van der Waals attraction force when $h = a_0$. The repulsive force arising from the mechanical contact of the tip with the sample surface is modeled using contact mechanics. Hence, the total force acting on the cantilever tip due to the adhesive and repulsive components is given by

$$F_{\text{contact}}(h) = -\frac{HR}{6a_0^2} + \frac{4}{3}E^*\sqrt{R}(a_0 - h)^{3/2} \quad \text{if } h < a_0$$

$$\frac{1}{E^*} = \frac{(1 - \nu_t)^2}{E_t} + \frac{(1 - \nu_s)^2}{E_s} \quad (4)$$

where E^* is the effective Young's modulus of the tip-sample pair, E_t and E_s are the elastic moduli of the tip and surface materials, ν_t and ν_s are the Poisson's ratios of the tip and the surface materials, respectively.

Combining the contact and non-contact forces, the interaction force F_{ts} between the tip and the surface can be expressed as

$$F_{ts}(h) = \begin{cases} -\frac{HR}{6h^2} & \text{if } h > a_0 \\ -\frac{HR}{6a_0^2} + \frac{4}{3}E^*\sqrt{R}(a_0 - h)^{3/2} & \text{else.} \end{cases} \quad (5)$$

4. SIMULINK model

Simulating the dynamical behavior of the cantilever alone does not help us to investigate the scan performance under Q control for different scan settings. We also developed the models of the individual scan components and integrated them with the model of the cantilever to perform end-to-end

scanning simulations. In addition to the cantilever model and its force interactions with the sample, the complete model of the scanning system (shown in figure 3(b)) includes the numerical models of the following physical components:

- Vibrometer*: The laser Doppler vibrometer (LDV) in the physical set-up is modeled as a block which differentiates the vibration signal (i.e. AC deflection of the cantilever) first and then outputs it after adding a time delay on it. This time delay is caused by the digital signal processing unit of the LDV and confirmed to be fixed for the operating frequency of the cantilever [13].
- RMS converter*: This block is used to compute the RMS of the vibration velocity. A built-in block (RMS in the SimPowerMechanics Library) is used for this operation and the RMS value of the input signal is calculated over a running window. In order to calculate the oscillation amplitude of the cantilever, the RMS of the velocity signal is multiplied by a proper gain K as shown in figure 3(b).
- PI scan controller*: This block is used to control the vertical movements of the computer controlled XYZ stage. It has an analog to digital converter that samples the error signal at a fixed sampling rate. A built-in block (*pid* controller) is utilized to actuate the XYZ stage based on the error in the peak-to-peak amplitude of the cantilever oscillations ($A_{\text{set}} - A$).
- XYZ stage*: In order to model the dynamics of the computer controlled XYZ nano stage used in the physical set-up, we have used a first-order transfer function with a time constant smaller than the sampling time of the PI controller. The vertical movements of the XYZ stage are represented as s_2 in figure 3.
- Adaptive Q controller*: This block is used to calculate the gain $G(t)$ which depends on the peak-to-peak oscillation amplitude of the cantilever. If $G(t)$ is set to a constant value, this block functions as a standard Q controller. In AQC, the gain is adjusted on the fly depending on the RMS value. The output of this block, $G(t)$, is used to scale the velocity signal first and then the scaled signal (F_{AQC}) is added on the drive signal in order to change the Q_{eff} of the cantilever.

In addition to the models of above components, the following blocks are used for regulating input-output operations:

(i) *Input profile*: This block generates the input surface profile as a function of time. In the case of scanning calibration steps with a constant height of h_s and width of w_s , the input profile s_1 is periodic with a period of $t_s = w_s/v_s$, where v_s is the scan speed. For the time interval $0 \leq t \leq t_s$, s_1 is given by

$$s_1 = \begin{cases} 0 & 0 \leq t < \frac{t_s}{2} \\ h_s & \frac{t_s}{2} < t \leq t_s. \end{cases} \quad (6)$$

(ii) *Output profile*: This is the block where the inverse of the movements of the XYZ stage (s_2) are recorded. Hence, this is the output of the scanning system. The output scan profile should exactly match the desired input profile (s_1) under ideal conditions.

In the model, the parameters Z_c , h and z represent the vertical position of the resting cantilever with respect to the reference plane in the absence of tip-sample interaction, the vertical separation distance between the cantilever tip and the sample surface, and the instantaneous vertical position of the oscillating cantilever with respect to its resting position, respectively (figure 3(a)).

5. Scanning simulations

In this section, we investigate AFM scanning under standard Q control first and then extend our work to show the benefits of AQC through numerical simulations. The numerical results for AQC are also validated by scanning experiments performed in our physical AFM set-up. In standard Q control, the gain G is set to a constant value prior to scanning in order to increase or decrease the Q_{eff} of the cantilever and is not altered during scanning. In AQC, the Q_{eff} of the cantilever is adjusted in real time depending on the surface profile by setting the gain G adaptively on the fly.

We first investigate the effect of the Q factor and stiffness of a cantilever probe on its sensitivity in scanning soft and stiff samples (relative to the substrate surface) through numerical simulations. For this purpose, we performed scanning simulations with a 10 nm high soft sample ($E_{\text{sample}} = 200$ MPa) lying on a stiffer substrate ($E_{\text{substrate}} = 10$ GPa). This is a typical scenario encountered when scanning soft samples in liquid where the Q factor of the cantilever is low due to the environmental damping. The simulations are repeated for three different cantilevers ($k = 0.05, 0.5$, and 5 N m⁻¹) for Q_{eff} varying from 10 to 800. All other parameters in the numerical model such as the PI controller gains, the material properties of the cantilever tip, scan speed, resonance frequency and free-air amplitude of the cantilever are kept constant throughout the simulations. As shown in figure 4(a), the apparent (measured) height of the scanned sample depends on Q_{eff} and cantilever stiffness. As Q_{eff} is increased and k is decreased, the apparent height approaches the actual value. Our numerical simulations show that scanning in an attractive regime using soft cantilevers with high Q_{eff} results in a better image quality. The sudden jumps to the actual value shown in figure 4(a) for $k = 0.05$ and 0.5 N m⁻¹ occur when the

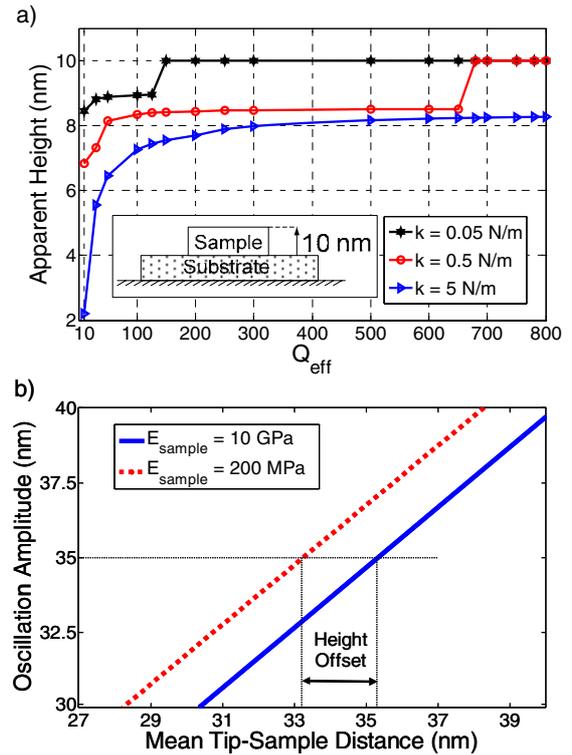


Figure 4. (a) Apparent height of a 10 nm sample ($E_{\text{sample}} = 200$ MPa) lying on a stiffer substrate ($E_{\text{substrate}} = 10$ GPa) for different values of effective quality factor and stiffness constant of the cantilever. (b) Oscillation amplitude versus mean tip-sample distance for samples having different elastic modulus ($A_{\text{set}} = 35$ nm, $A_0 = 50$ nm).

cantilever starts to operate in the attractive regime. In this regime, only the non-contact forces are effective. The probe is not tapping on the sample surface and oscillation amplitude is reduced only by the non-contact interactions [19]. Since the probe tip is not in physical contact with the sample surface during this period, there is no sample deformation and hence no difference between the measured and actual heights of the sample.

If the scanning is performed in the repulsive regime, where the cantilever tip touches the sample surface, the offset between the measured and actual heights is more prominent, especially for stiffer cantilevers. In this regime, the contact mechanics dominates the interactions between the probe tip and the sample surface. Hence, the elastic moduli of the cantilever tip and sample both influence the scan quality. In figure 4(b), we show the change in the oscillation amplitude of a cantilever probe as a function of the tip-sample distance when the probe tip interacts with soft ($E_{\text{sample}} = 200$ MPa) and stiff samples ($E_{\text{sample}} = 10$ GPa) lying on a stiff substrate ($E_{\text{substrate}} = 10$ GPa). The cantilever tip indents more into the soft sample than it does into the stiffer one to reach the same set amplitude and hence a height offset in the order of nanometers occurs when scanning soft samples. From the numerical simulations, we observe that this problem is more pronounced if the Q_{eff} of the cantilever is low, as occurs when the probe is immersed into liquid. These numerical simulations show

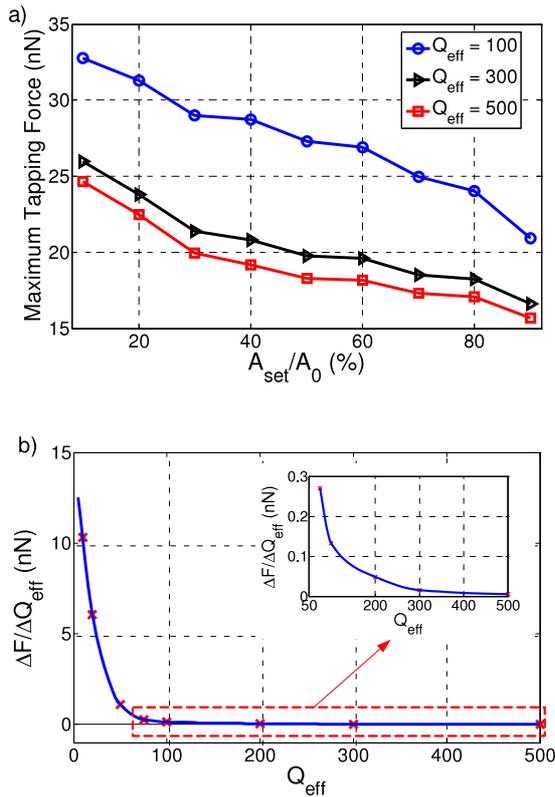


Figure 5. (a) Maximum tapping forces as a function of effective quality factor for different set amplitudes. (b) The rate of change in tapping forces as a function of effective quality factor for $A_{set}/A_0 = 70\%$. The elastic modulus of the sample and the substrate are taken as 179 GPa.

a good agreement with the experimental studies of Ebeling *et al* [22] and Humphris *et al* [5]. In both of those studies, an increase in the apparent height of DNA on mica is reported when the effective quality factor of the cantilever is enhanced. In the case of scanning samples as stiff as the substrate surface, the height offset becomes insignificant. Although the scanning is performed in the repulsive regime, the indentation of the probe tip into the sample surface is minimal throughout the sample surface independent of the stiffness of the cantilever.

Secondly, we consider the effect of Q factor on the tapping forces. In addition to the material properties of the sample, the force interactions between the probe tip and the sample surface depend on the free-air oscillation amplitude A_0 and the set amplitude A_{set} of the probe when scanning under Q control. We performed numerical simulations to investigate the effect of A_{set} (as a percentage of A_0) and Q_{eff} on the tapping forces. In figure 5(a), we present the magnitude of the maximum tapping force as a function of A_{set}/A_0 for different values of Q_{eff} . The maximum tapping force is calculated using the average of maximum indentations of the probe tip into the sample surface after the tapping amplitude reaches steady state (i.e. $A = A_{set}$). As A_{set}/A_0 approaches 1, the probe tip starts tapping the sample surface lightly and the resultant interaction forces decrease. Similarly, as Q_{eff} increases, the tapping forces also decrease. However, for a given A_{set}/A_0 , the rate of decrease in tapping forces is less significant at higher values of Q_{eff} (figure 5(b)). For scanning soft samples in liquid,

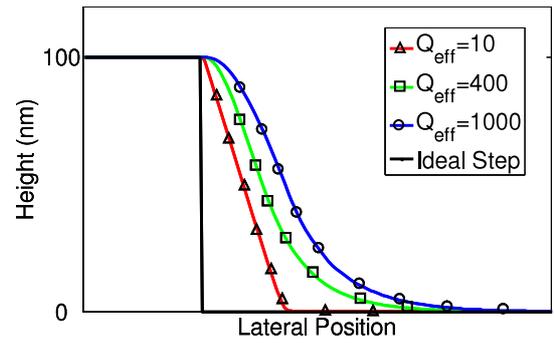


Figure 6. Scanning a downward step using a cantilever probe having different values of effective quality factor. The elastic moduli of the sample and the substrate are taken as 70 and 179 GPa, respectively.

keeping the tapping forces low is crucial in order to prevent damage to the sample. It is also desired to have lower tapping forces to prevent tip wear during the scanning of stiffer surfaces in air as well.

Increasing the Q factor, especially when operating in liquid, has the benefits of decreasing the tapping forces and improving the sensitivity of the probe such that soft samples can be traced better. However, if the sample surface is stiffer and the native Q factor of the cantilever probe is already high, which is typically the case when scanning in air, the probe sensitivity has a limited influence, but its slow transient response adversely affects the image quality. The bandwidth of the cantilever, that is how fast it responds to the changes in surface profile, is inversely proportional to its Q factor. As a result, increasing the Q factor limits the maximum achievable scan speed [11, 12]. In order to show the effect of the Q factor of a cantilever on its bandwidth and in return on the maximum achievable scan speed, we present the simulation results of scanning a 100 nm step for three different values of $Q_{eff} = 10, 400$ and 1000 (figure 6). As the Q_{eff} is increased, the response of the probe to the rapid changes in surface profile becomes slower and it cannot trace the input profile well. As shown in figure 6, it takes longer time for the cantilever to return to the set amplitude when a downward step is encountered (figure 6).

Therefore, there is a trade-off between the maximum achievable scan speed and the tapping forces applied to the sample when scanning under Q control. Higher Q values promote lower tapping forces while lower ones result in an increased scanning speed. In order to show this trade-off quantitatively, we performed simulations for different values of A_{set} and scan speeds. We have defined an error measure to evaluate and compare the scan performances under different scan settings. This measure is based on the positional error between the measured (output) and desired (input) scan profiles. We first define e_x as the absolute value of the positional difference between the measured and actual heights of the sample surface at a lateral position x along a scan line. Then, the total scan error, e_s , is calculated by integrating the positional error e_x over the scan line. The magnitude of the scan error is zero if the resultant scan profile exactly matches the actual surface profile. In the case of scanning calibration

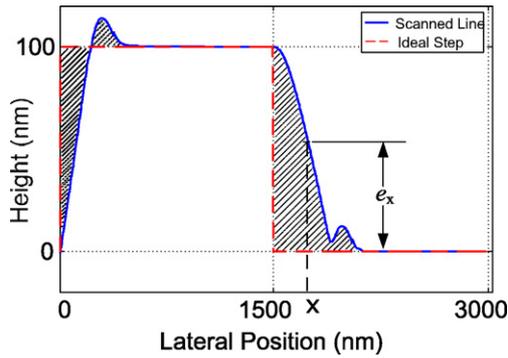


Figure 7. Scan profile (blue solid line) of an ideal step (red dashed line) with a height of $h_s = 100$ nm and width of $w_s = 3 \mu\text{m}$.

steps with a constant height of h_s (figure 7), the total scan error is calculated by first integrating the positional error e_x over a full step width w_s and then normalizing the sum by the area under the step. This normalization makes the scan error invariant of the scan speed so that it can be used for comparing the results of different scan speeds. Hence, the scan error e_s is calculated as

$$e_s = \frac{\int_0^{w_s} |e_x| dx}{w_s h_s}. \quad (7)$$

In figure 8, we present the iso-error curves obtained by scanning a 100 nm step under Q control for $Q_{\text{eff}} = 100$ and 500. It is observed that the scan error increases as the scan speed and A_{set} increase. Also, increasing the Q factor of the cantilever causes higher scan errors. However, recall that tapping forces are reduced as the Q factor is increased (figure 5(a)). The influence of A_{set} on this trade-off becomes more prominent when operating at higher scan speeds (iso-error lines become more inclined at higher scan speeds in figure 8).

In figure 9, we compare the performance of standard Q control and AQC using iso-error lines. For a fixed scan error of $e_s = 20\%$ and $A_{\text{set}}/A_0 = 70\%$, one can easily reach higher scan speeds using AQC for $Q_{\text{eff}} = 300$. As shown in the figure, one can also reach similar scan speeds by setting the Q factor to $Q_{\text{eff}} = 5$ using standard Q control, but this causes an increase of approximately nine times in the maximum tapping force applied to the sample when it is compared to case of AQC for $Q_{\text{eff}} = 300$.

6. Experiments

While the tapping forces are reduced as the Q factor is increased, the transient response of the probe becomes slower and hence the error signal saturates for a longer period of time, limiting the maximum achievable speed. For example, when scanning steps with a constant height, the error saturation occurs at the beginning and also at the end of the step. When an upward step is encountered, the probe tip suddenly sticks to the surface, the oscillation amplitude reduces to zero and the error signal ($A_{\text{set}} - A$) saturates at A_{set} (see the error signal between the lateral positions p1 and p2 in figure 10). When a sharp downward step is encountered, the oscillation amplitude

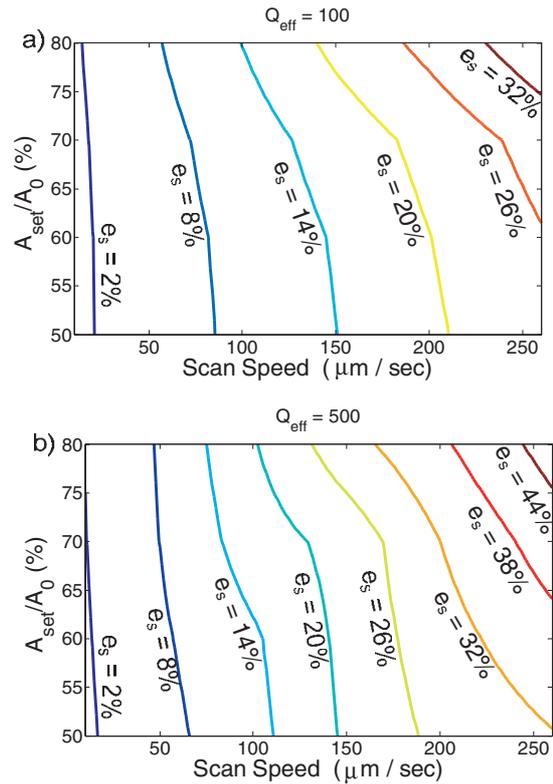


Figure 8. Iso-error curves for the scan results of a 100 nm step for (a) $Q_{\text{eff}} = 100$ and (b) $Q_{\text{eff}} = 500$.

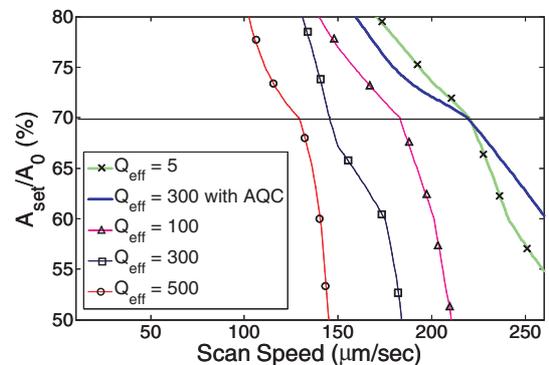


Figure 9. Comparison of standard Q control and AQC using iso-error curves for the scan error of $e_s = 20\%$.

of the probe reaches its free-air value and the error signal this time saturates at $A_{\text{set}} - A_0$ (see the error signal between the lateral positions p3 and p4 in figure 10). Choosing a high value for A_{set} reduces the saturation problem at the beginning of the step (since the magnitude of the error signal is high, the controller responds more rapidly) and also reduces the tapping forces (figure 5(a)), but amplifies the saturation problem at the end of the step. These saturations result in an inclined profile at the entrance and exit of the step (see scan profiles in figure 10).

The error saturation is also adversely affected by the increase in scan speed. This, in fact, limits the maximum achievable scan speed. In figures 11(a) and (c), we present the

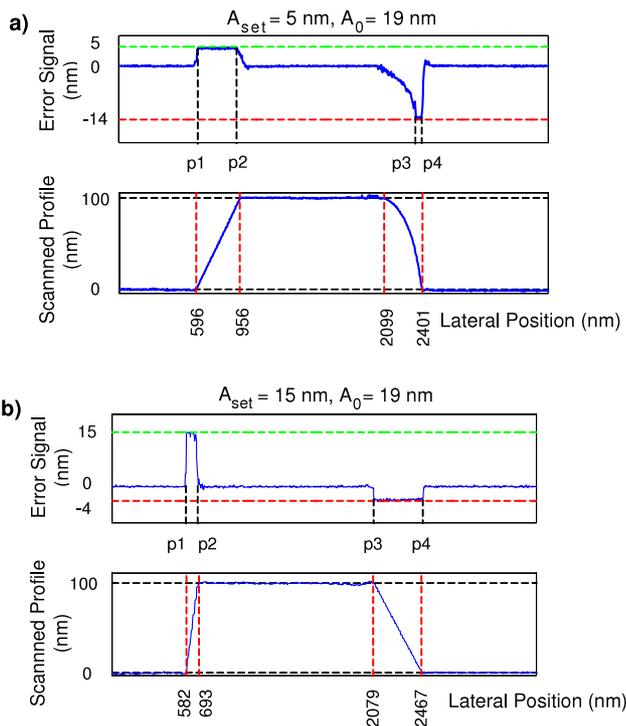


Figure 10. The experimental results of scanning 100 nm calibration steps at two different settings of $A_{set} = 5$ nm and 15 nm ($A_0 = 19$ nm). The lateral positions where the error saturation occurs are p1–p2 and p3–p4.

experimental results of scanning 100 nm calibration steps using a conventional PI scan controller for two different scan speeds of 2 and 10 $\mu\text{m s}^{-1}$, respectively. The other scan parameters are kept constant during the experiments and hence the elapsed time during error saturations are the same at both scan speeds. However, the lateral distance traveled during the error saturated period is different, resulting in a less accurate scan profile for the faster scan (figure 11(c)). Therefore, the error saturation is a major problem limiting the maximum achievable scan speed when scanning surfaces having sharp changes in topography. The saturation problem is also observed in the numerical simulations, and the scan profiles obtained through numerical simulations (figures 11(b) and (d)) show a good agreement with the experimental ones.

The AQC reduces the error saturation problem and increases the maximum achievable scan speed while the increase in tapping forces is minimal (figure 11(e)). As an alternative, the integral gain constant of the PI controller can be increased to overcome the saturation problem [23]. However, there is an upper limit for its value. A higher controller gain magnifies the noise in the measurement (i.e. the cantilever deflection signal) and significantly reduces the quality of the resultant image.

As can be seen from figure 11(e), the cantilever probe tracks the input profile better in AQC, resulting in a sharper image. In AQC, the Q factor of the probe is set to an initial value as in standard Q control, but then modified on the fly during scanning when necessary. For example, if an error saturation is detected when scanning a downward step, AQC

	Physical Experiments	Numerical Simulations
2 $\mu\text{m/sec}$ PI Controller		
10 $\mu\text{m/sec}$ PI Controller		
10 $\mu\text{m/sec}$ PI Controller + AQC		

Figure 11. The results of the experimental and numerical scans without AQC for scan speeds of 2 $\mu\text{m s}^{-1}$ ((a) and (b)) and 10 $\mu\text{m s}^{-1}$ ((c) and (d)) and with AQC for scan speed of 10 $\mu\text{m s}^{-1}$ ((e) and (f)). More experimental results comparing standard and adaptive Q control are available in our earlier publication [13].

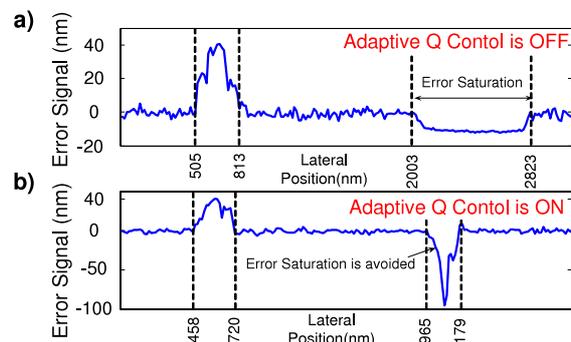


Figure 12. The error signal recorded during the scanning of 100 nm calibration steps (scan speed = 10 $\mu\text{m s}^{-1}$) when the adaptive Q controller is turned off and on. The error saturation observed in (a) is avoided using AQC (b).

automatically increases the gain G (and hence the Q factor of the probe). This saturation occurs when $A > A_{threshold}$, where $A_{threshold}$ is a threshold value close to A_0 . An increase in the Q factor causes an increase in the vibration amplitude A as well as the magnitude of the error signal (figure 12), which results in a faster response of the z -actuator moving the sample. As a result, the adverse effects of the error saturation on the output profile are significantly reduced using AQC. Moreover, since the free-air saturation problem is suppressed using AQC, one can use a higher A_{set} to reduce the tapping forces as well as the error saturation at the beginning of the step, as discussed earlier.

7. Discussion and conclusions

The trade-off in setting the Q factor of a cantilever probe was investigated numerically and the performance of standard Q control was quantitatively compared to that of AQC using a new error measure. This error measure is based on the physical dimensions of the surface being scanned only and for someone interested in the material properties of the sample, it does not help to compare different scans. The results of the numerical simulations were validated through scan experiments performed in a physical set-up. Although numerical simulations have been performed in the past to investigate the cantilever dynamics and tip-sample interactions, only a few recent studies have focused on the simulation of whole scan process [14]. Since it is almost impossible to repeat a scan experiment under exactly the same conditions in real world settings due to variations in humidity, electrical noise, ground vibrations, temperature, etc, the development of numerical simulations is important. Moreover, even if the experimental conditions are fixed, the probe tip or the sample surface may get damaged in time, affecting the scan results adversely. All these factors make it impossible to quantitatively compare the results of experimental scans under different scan settings. On the other hand, we, for example, easily constructed the performance lines of constant error for different scan settings using numerical simulations to compare the performance of standard Q control with AQC in our study. In addition, we readily accessed all the outputs of the simulations, some of which are not directly measurable in physical experiments (e.g. the magnitude of maximum tapping forces shown in figure 5).

Moreover, one can also easily run 'what-if' scenarios in a simulation world to investigate the scan performance not only for different settings of scan parameters but also for different scan environments such as liquid and air. For example, we investigated the effect of stiffness constant and Q factor of a cantilever on the scan profile when scanning a soft sample lying on a stiffer substrate (figure 4). We showed that scanning in an attractive regime using soft cantilevers having high Q_{eff} results in a better image quality. If a soft sample (relative to the substrate surface) is scanned in liquid where the Q factor drops significantly, the probe tip cannot accurately trace the surface profile and the height of the sample surface is measured to be less than its actual value. Moreover, there is a risk of damaging the sample due to high tapping forces at low values of Q (figure 5(a)). To overcome these problems, the Q factor of the cantilever is increased when scanning in liquid. On the other hand, when scanning in air, the native Q factor of the cantilever is typically high, and increasing it further does not significantly reduce the tapping forces. Our simulation results show that the magnitude of tapping forces is high at low values of Q_{eff} and decreases as the Q_{eff} is increased while the rate of drop is not significant at higher values (figure 5(b)). Moreover, the slow transient response of the cantilever at high values of Q_{eff} limits the maximum achievable scan speed. Hence, reducing the Q factor increases the scan speed, but it also increases the magnitude of tapping forces, which may cause damage to the sample and/or the probe tip. However, it is possible

to achieve higher scan speeds using AQC without causing an increase in the tapping forces (figure 9). We showed that error saturation is the major problem limiting the scan speed in tapping mode AFM under standard Q control and AQC solves this problem (figure 12). In AQC, if there is a tendency towards saturation in the error signal due to the rapid variations in surface topography, the controller changes the Q factor of the probe instantaneously to avoid the saturation problem. Moreover, since the error saturation problem is suppressed, one can set higher values of A_{set} to reduce the tapping forces as well (see the relation in figure 5(a)).

References

- [1] Zhong Q, Imniss D, Kjoller K and Elings V B 1993 Fractured polymer/silica fiber surface studied by tapping-mode atomic force microscopy *Surf. Sci.* **290** 688
- [2] Anczykowski B, Cleveland J P, Krüger D, Elings V B and Fuchs H 1998 Analysis of the interaction mechanisms in dynamic mode SFM by means of experimental data and computer simulation *Appl. Phys. A* **66** S885
- [3] Tamayo J, Humphris A D L, Owen R J and Miles M J 2001 High- Q dynamic force microscopy in liquid and its application to living cells *Biophys. J.* **81** 526
- [4] Grant A and McDonnell L 2003 A non-contact mode scanning force microscope optimized to image biological samples in liquid *Ultramicroscopy* **97** 177
- [5] Humphris A D L, Round A N and Miles M J 2001 Enhanced imaging of DNA via active quality factor control *Surf. Sci.* **491** 468
- [6] Rodríguez T R and García R 2003 Theory of Q control in atomic force microscopy *Appl. Phys. Lett.* **82** 4821
- [7] Kokavecz J, Horvath Z L and Mechler A 2004 Dynamical properties of the Q -controlled atomic force microscope *Appl. Phys. Lett.* **85** 3232
- [8] Hoscher H, Ebeling D and Schwarz U D 2006 Theory of Q -controlled dynamic force microscopy in air *J. Appl. Phys.* **99** 084311
- [9] Jäggi R D, Franco-Obregón A, Studerus P and Ensslin K 2001 Detailed analysis of forces influencing lateral resolution for Q -control and tapping mode *Appl. Phys. Lett.* **79** 135
- [10] San Paulo A and García R 2002 Unifying theory of tapping-mode atomic force microscopy *Phys. Rev. B* **66** 041406
- [11] Sulchek T, Hsieh R, Adams J D, Yaralioglu G G, Minne S C, Quate C F, Cleveland J P, Atalar A and Adderton D M 2000 High-speed tapping mode imaging with active Q control for atomic force microscopy *Appl. Phys. Lett.* **76** 1473
- [12] Sulchek T, Yaralioglu G G, Quate C F and Minne S C 2002 Characterization and optimization of scan speed for tapping-mode atomic force microscopy *Rev. Sci. Instrum.* **73** 2928
- [13] Gunev I, Varol A, Karaman S and Basdogan C 2007 Adaptive Q control for tapping-mode nanoscanning using a piezoactuated bimorph probe *Rev. Sci. Instrum.* **78** 043707
- [14] Kowalewski T and Legleiter J 2006 Imaging stability and average tip-sample force in tapping mode atomic force microscopy *J. Appl. Phys.* **99** 064903
- [15] Schitter G, Menold P, Knapp H F, Allgöwer F and Stemmer A 2001 High performance feedback for fast scanning atomic force microscopes *Rev. Sci. Instrum.* **72** 3320
- [16] San Paulo A and García R 2001 Tip-surface forces, amplitude, and energy dissipation in amplitude-modulation (tapping mode) force microscopy *Phys. Rev. B* **64** 193411

- [17] Perez R, Stich I, Payne M C and Terakura K 1998 Surface–tip interactions in noncontact atomic-force microscopy on reactive surfaces: Si(111) *Phys. Rev. B* **58** 10835
- [18] García R and San Paulo A 1999 Attractive and repulsive tip–sample interaction regimes in tapping-mode atomic force microscopy *Phys. Rev. B* **60** 4961
- [19] Aimé J P, Boisgard R, Nony L and Couturier G 1999 Nonlinear dynamic behavior of an oscillating tip–microlever system and contrast at the atomic scale *Phys. Rev. Lett.* **82** 3388
- [20] Israelachvili J 1995 *Intermolecular and Surface Forces* (London: Academic)
- [21] Derjagurin B V, Muller V M and Toporov Y P 1975 Effects of contact deformations on the adhesion of particles *J. Colloid Sci.* **53** 314
- [22] Ebeling D, Hölscher H, Fuchs H, Anczykowski B and Schwarz U D 2006 Imaging of biomaterials in liquids: a comparison between conventional and Q -controlled amplitude modulation ('tapping mode') atomic force microscopy *Nanotechnology* **17** S221
- [23] Kodera N, Sakashita M and Ando T 2006 Dynamic proportional-integral-differential controller for high-speed atomic force microscopy *Rev. Sci. Instrum.* **77** 083704