Chapter 14
Amplitude Modulation (AM) Mode in Dynamic Atomic Force Microscopy

In dynamic atomic force microscopy the cantilever is excited using a piezo actuator which oscillates the cantilever base. The driving frequency is usually close to the resonance frequency of the cantilever. Due to the interaction between tip and the surface, the resonance frequency of the cantilever changes. As shown in this chapter, an attractive force between tip and sample leads to a lower resonance frequency of the cantilever, while for repulsive tip-sample forces the resonance frequency increases.[1]

This change in resonance frequency can be measured directly in the so called frequency modulation mode (FM) of atomic force microscopy, as described in Chap. 17. In this chapter, we describe the amplitude modulation mode (AM) of AFM. Here the cantilever is driven at a fixed frequency with a fixed driving amplitude. The change of the resonance frequency leads to a change of the vibration amplitude and of the phase between excitation and oscillation, which can be measured.

We consider the AM detection mode in this chapter in the small amplitude limit in which the tip-sample force is approximated as linear in the range of the oscillation amplitude. In this case, the AM detection mode can be treated analytically. While in practice the AM detection mode is rarely used in this limit, the basic concepts can be explained more easily using this limit. When in the next chapter the small amplitude limit is lifted, things become somewhat more complicated. However, armed with a basic understanding obtained from the treatment of the small amplitude limit, the more complicated case is then easier to comprehend.

14.1 Parameters of Dynamic Atomic Force Microscopy

Compared to STM which has only two parameters, the tunneling current and the tunneling voltage, there are many more parameters in dynamic AFM.

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[1] Actually, this is not strictly true: As shown later it is not the sign of the force, but rather the sign of the *force gradient* that determines the direction of the resonance frequency shift.

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- The resonance frequency of the free cantilever ω_0
- The force constant of the cantilever k
- The quality factor of the cantilever Q_{cant}
- The driving amplitude of the oscillation A_{drive}
- The oscillation amplitude A
- The phase ϕ between driving and oscillation
- The driving frequency ω_{drive}
- The frequency shift of the resonance frequency $\Delta\omega$ relative to ω_0 due to a tip-sample interaction

The first two parameters are given by the cantilever, while the Q-factor depends on the cantilever and also on the operating environment (ambient or vacuum). Depending on the operating mode, further parameters can be set by the operator or measured:

- In AM detection the amplitude A and phase ϕ of the oscillation are measured, while ω_{drive} and A_{drive} are set.
- In FM detection the shift of the resonance frequency $\Delta\omega$ is measured.

Because this multitude of parameters may seem somewhat discouraging, we will discuss the parameters and the relations among them step by step in the following.

14.2 Principles of Dynamic Atomic Force Microscopy I (Amplitude Modulation)

As the simplest model for the cantilever under the influence of a tip-sample interaction, we consider the driven damped harmonic oscillator as discussed in Sect. 2.3 including the influence of a time-independent external force F_{ts}, which depends on the tip-sample distance. In this section, we assume that dissipation enters only via the (air) damping of the cantilever, while the tip-sample interaction is assumed to be conservative.

We assume the limit of small amplitude, which means that F_{ts} varies only slowly in the range of the oscillation amplitude A. In this case, F_{ts} will be approximated as linear in the following. We use this limit here because this idealized scenario can be solved analytically. For the usual vibration amplitudes (several nanometers) the small amplitude limit does not hold.

The definition of the coordinates of the cantilever-tip-sample system is given in Fig. 14.1. For the tip oscillation, we use the coordinate z. For the tip-sample force $F_{\text{ts}}(d+z)$, we use the coordinate $d+z$ (tip-sample distance), with the offset d being the average tip-sample distance during an oscillation cycle.

Due to the small amplitude assumption, we can expand the force $F_{\text{ts}}(d+z)$ around the equilibrium position of the tip ($z=0$, corresponding to a tip-sample distance d) as

$$F_{\text{ts}}(d+z) = F_{\text{ts}}(d) + \left.\frac{\partial F_{\text{ts}}}{\partial z}\right|_{z=0} z + \cdots . \tag{14.1}$$

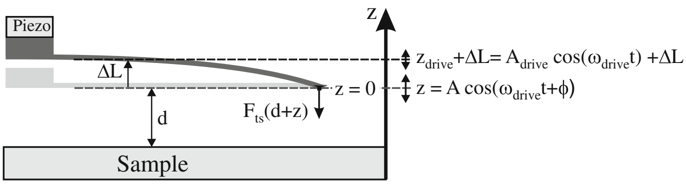

Fig. 14.1 Definition of the coordinates for a driven damped harmonic oscillator under the influence of a tip-sample force

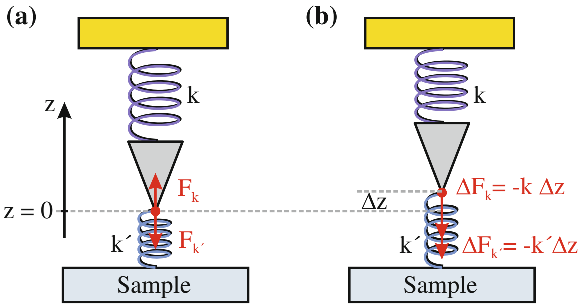

Fig. 14.2 **a** For the case of small amplitudes, the cantilever-tip-sample system can be effectively described by two springs, one representing the cantilever with force constant k and one representing the tip-sample interaction with force constant k'. **b** This system is equivalent to a system with an effective spring constant of $k_{\text{eff}} = k + k'$

In this approximation the force changes linearly with z, like it is the case for a spring. Hence the influence of the tip-sample force can be described by a spring with a spring constant k' equal to the negative force gradient, as

$$k' = -\frac{\partial F_{\text{ts}}}{\partial z}\bigg|_{z=0}. \tag{14.2}$$

The tip-sample interaction can be represented by adding a small spring with spring constant $k' \ll k$, as shown in Fig. 14.2a. The two spring constants add up[2] to an effective spring constant $k_{\text{eff}} = k + k'$. However, this analogy (replacing the tip-sample interaction by a spring) should not be stretched too far, since real spring constants of springs are always positive, while a tip-sample interaction can also have

[2] Since the two springs attach to the tip from above and below one might think that this should lead to a subtraction of the spring constants. Here we show that the spring constants indeed add up. As indicated in Fig. 14.2 the cantilever spring under the influence of a tip-sample force can be replaced by a cantilever effective mass held by two springs. In static equilibrium, $z = 0$, the forces of both springs compensate as $F_k + F_{k'} = 0$. If the cantilever is moved by Δz during the oscillation, Fig. 14.2b shows that the force components relative to the forces in static equilibrium point in the same direction for both springs and $\Delta F = \Delta F_k + \Delta F_{k'} = -(k + k')\Delta z$ results. Thus the spring constants k and k' combine to $k_{\text{eff}} = k + k'$.

a "negative spring constant". Such a negative spring constant k' cannot be realized by a coil spring or a cantilever-shaped spring, but can exist in a more general sense as a potential of negative curvature.

Before we analyze the harmonic oscillator with the spring constant k_{eff}, we consider the static case (i.e. all oscillatory amplitudes in Fig. 14.1 are zero). Without a sample being present, the tip is at its zero position $z = 0$ and the cantilever is unbent (shown in light gray in Fig. 14.1). In this case the static bending ΔL is zero.[3] If the sample is now brought close to the tip, the tip-sample interaction will change the tip position. Since we would like to probe the sample at a (tip-sample) distance d, the initial zero position of the tip, $z = 0$, is restored by moving the cantilever base in the opposite direction, shown in dark gray in Fig. 14.1. In static equilibrium with the cantilever bent, the tip-sample force and the static bending force balance at $z = 0$ as

$$F_{\text{ts}}(d) = -k_{\text{eff}} \Delta L, \tag{14.3}$$

with ΔL being the static (offset) deflection of the cantilever as indicated in Fig. 14.1.

We will now consider a sinusoidal excitation of the cantilever base at the frequency ω_{drive} and amplitude A_{drive} around the position of static equilibrium as $z_{\text{drive}} = A_{\text{drive}} \cos(\omega_{\text{drive}} t)$. As a result of this excitation, the tip will oscillate in the steady-state around its equilibrium position as $z = A \cos(\omega_{\text{drive}} t + \phi)$. This case corresponds to the driven damped harmonic oscillator discussed in Sect. 2.3 and using (2.17) the equation of motion can be written as

$$\ddot{z} + \sqrt{\frac{k_{\text{eff}}}{m}} \frac{1}{Q_{\text{cant}}} \dot{z} + \frac{k_{\text{eff}}}{m} (z - z_{\text{drive}}) = 0. \tag{14.4}$$

The tip-sample force is included by replacing the spring constant k by k_{eff}. As the force $F_{\text{ts}}(d)$ cancels out the force due to the static bending of the cantilever $-k_{\text{eff}} \Delta L$, according to (14.3), these terms have already be removed from the equation of motion. The equation of motion (14.4) was solved in Sect. 2.3 with the result that a resonance occurs at $\omega_0 = \sqrt{k/m}$. Since we replaced k by the effective spring constant k_{eff} in order to include the effect of a tip-sample force, the resonance frequency will shift from ω_0 for the case without tip-sample interaction to $\omega_0' = \sqrt{k_{\text{eff}}/m}$. Thus

$$\omega_0' = \sqrt{\frac{k_{\text{eff}}}{m}} = \sqrt{\frac{k + k'}{m}} = \sqrt{\frac{k}{m}\left(1 + \frac{k'}{k}\right)} = \omega_0 \sqrt{1 + \frac{k'}{k}}. \tag{14.5}$$

In the following, we assume that $|k'| \ll k$. For small x the approximation $\sqrt{1+x} \approx 1 + \frac{1}{2}x$ holds. Therefore, the new resonance frequency of the cantilever can be written as

$$\omega_0' \approx \omega_0 \left(1 + \frac{k'}{2k}\right). \tag{14.6}$$

[3] The tip length is set to zero in order to avoid an additional offset length.

The shift of the resonance frequency results in

$$\Delta\omega = \omega_0' - \omega_0 = \omega_0 \frac{k'}{2k} = -\frac{\omega_0}{2k} \frac{\partial F_{\mathrm{ts}}}{\partial z}\bigg|_{z=0}. \tag{14.7}$$

This result can be easily related to the experimentally observed frequency shift Δf as

$$\Delta f = \frac{\omega_0' - \omega_0}{2\pi} = f_0 \frac{k'}{2k} = -\frac{f_0}{2k} \frac{\partial F_{\mathrm{ts}}}{\partial z}\bigg|_{z=0}. \tag{14.8}$$

Together with the resonance frequency (maximum of the resonance curve) also the whole resonance curve shifts by Δf. In summary, the frequency shift of the resonance curve induced by the tip-sample interaction is proportional to the (negative) gradient of the tip-sample force ($F_{\mathrm{ts}}'(d) = \partial F_{\mathrm{ts}}(d + z)/\partial z|_{z=0}$) if the following conditions are fulfilled: (a) The tip-sample force can be approximated as linear in the range of the oscillation amplitude, and (b) the tip-sample force gradient is much smaller than the spring constant of the cantilever $|k'| \ll k$ (the spring constant of the cantilever k is always positive).

The small amplitude limit and its interpretation in terms of the effective spring constant is also summarized in Fig. 14.3. A Lennard-Jones type force is shown together with the tip oscillation path with amplitude A around the average tip-sample distance d. The cantilever force $F_{\mathrm{cant}} = -kz$ is shown as a green line. The tip-sample force is approximated locally around $z = 0$ as linear $\Delta F_{\mathrm{ts}} = -k'z = \partial F_{\mathrm{ts}}/\partial z|_{z=0}\, z$, which is indicated by the dashed blue line. The resulting total force is shown as a red line with a slope of $k_{\mathrm{eff}} = k + k'$. Since $k' < 0$ and $|k'| \ll k$, the spring constant of the cantilever spring constant k is reduced by $|k'|$ comparing the green and red lines.

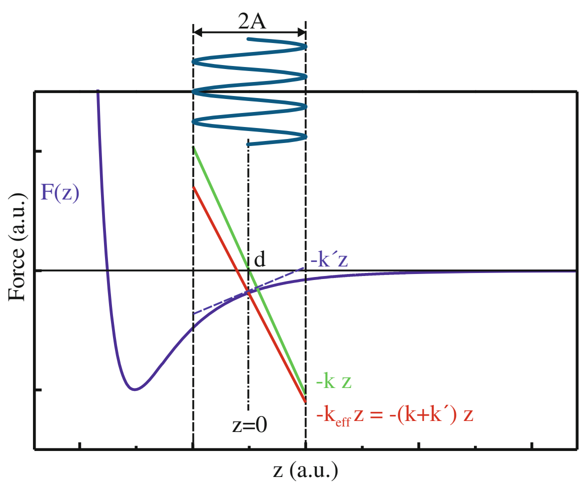

Fig. 14.3 In the small amplitude limit, the tip-sample force is approximated as linear within the range of the oscillation proportional to $-k'$. In this figure $k' < 0$ at the tip-sample distance d and the cantilever spring constant k is always positive. Thus the total effective force constant is the cantilever spring constant k reduced by the tip-sample force gradient proportional to k'

For a positive tip-sample force gradient $\partial F_{ts}/\partial z = -k' > 0$ the resonance frequency will shift to lower values $\Delta f < 0$, while for a negative force gradient $\partial F_{ts}/\partial z = -k' < 0$ the resonance frequency will shift to higher values $\Delta f > 0$. The frequency shift does not depend on the constant static offset force $F_{ts}(d)$. This offset force results only in a static deflection of the cantilever, which is compensated by an offset shift of the cantilever base by ΔL, according to (14.3).

Often it is stated slightly imprecisely that the frequency shift Δf is positive (towards higher frequencies relative to ω_0) for repulsive forces and negative for attractive forces. We can understand this if we have a closer look at Fig. 14.4, where the potential, the force, and the (negative) force gradient are shown. Here again the Lennard-Jones potential is considered as a model for the tip-sample interaction. The border between the repulsive and attractive regime is located at the zero of the force (dotted line in Fig. 14.4). Correspondingly, the border between the positive and negative force gradient is shown by a dashed line. For the largest range of tip-sample distances, the force and the negative force gradient (green and blue curves in Fig. 14.4, respectively) have the same sign. Only for a small range of distances (shaded gray in Fig. 14.4) do the tip-sample force and the negative force gradient have a different sign. As discussed above, the frequency shift Δf is proportional to the *negative* force gradient (14.8). Correspondingly, attractive forces (negative sign) lead (in the majority of cases—except in the gray-shaded range) to a decrease of the resonance frequency. Thus the statement that the frequency shift Δf is positive (towards higher frequencies) for repulsive forces and negative for attractive forces is true for most tip-sample distances.

The relative frequency change can be written as

$$\frac{\Delta f}{f_0} = \frac{k' A^2}{2k A^2} = \frac{E_{\text{interaction}}}{2E_{\text{cantilever}}}. \tag{14.9}$$

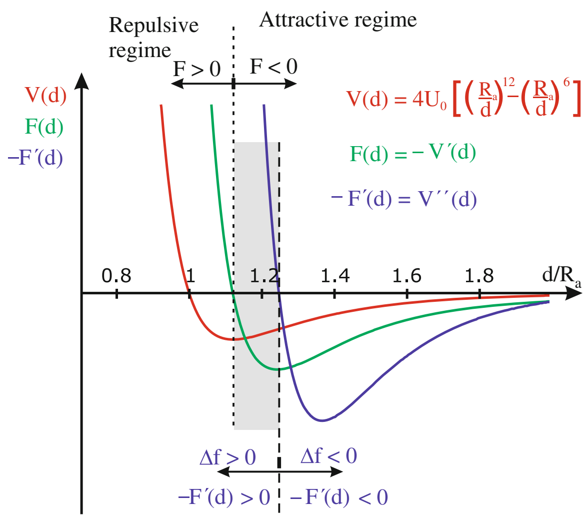

Fig. 14.4 Potential, force and negative force gradient for the Lennard-Jones model potential shown as a function of the average tip-sample distance d. As the frequency shift Δf is proportional to the negative force gradient it can be stated: For distances outside the *shaded region* the frequency shift Δf is positive (towards higher frequencies relative to ω_0) for repulsive forces, and negative for attractive forces

This means that the relative frequency shift is given by the ratio of the energy of the tip-sample interaction (spring constant k') divided by twice the energy stored in the cantilever oscillation (spring constant k).

14.3 Amplitude Modulation (AM) Detection Scheme in Dynamic Atomic Force Microscopy

We have seen that in the small amplitude limit a force gradient of the tip-sample interaction shifts the resonance frequency ω_0 by $\Delta\omega$. Accordingly, the whole resonance curve shifts by $\Delta\omega$ relative to that of the free cantilever, as shown in Fig. 14.5b.

In the amplitude modulation (AM) detection scheme, the cantilever is excited with a fixed driving amplitude A_{drive} at a fixed frequency ω_{drive} close to the resonance frequency. The resulting cantilever oscillation amplitude A is measured. As shown in Fig. 14.5, this amplitude depends indirectly on the tip-sample distance. The amplitude depends on the frequency shift of the resonance curve, which depends on the force gradient, which depends in turn on the tip-sample distance as $A(\Delta\omega(F'_{\text{ts}}(d)))$.

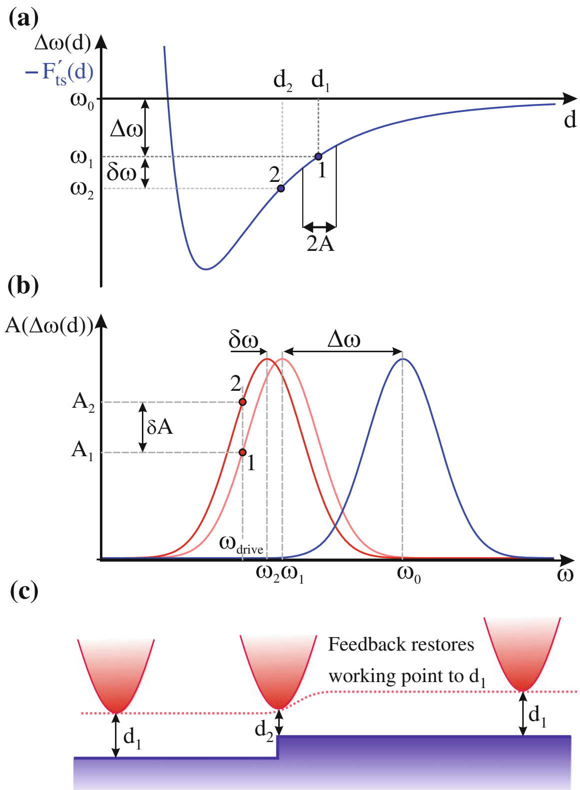

Fig. 14.5 In dynamic AFM the measured signal depends indirectly on the tip-sample distance. **a** Primarily, the force gradient and therefore also the resonance frequency (shift) depend on the tip-sample distance (here a Lennard-Jones potential is assumed). **b** Secondly, the measured amplitude depends on the frequency shift. For clarity $\Delta\omega_0$ has been chosen to be large compared to the width of the resonance curve. **c** When scanning over a step edge, the tip-sample distance changes until the feedback restores the old tip-sample distance

In the following, we go through these dependence step by step. The dependence of the force gradient on the tip-sample distance $F'_{ts}(d)$ based on the Lennard-Jones model potential is shown in Fig. 14.5a. As discussed in the previous section, the frequency shift is proportional to the force gradient indicated by the double labeling of the ordinate in Fig. 14.5a. In Fig. 14.5b resonance curves $A(\omega)$ are shown which are shifted together with the respective resonance frequency. The actual oscillation amplitude of the cantilever at the driving frequency is the measurement signal. In the feedback loop for the amplitude signal, a setpoint amplitude is selected, e.g. A_1 in Fig. 14.5b. The feedback loop controls the measured amplitude to the setpoint value by changing the z-position of the sample. This changes the tip-sample distance, which changes the force gradient, which changes the resonance frequency, and thus indirectly the amplitude is ultimately changed and kept at its setpoint value. If the feedback loop maintains a constant oscillation amplitude throughout a scan, this corresponds to a height profile taken at constant force gradient. Due to the dependence of the amplitude on the slope of the resonance curve the AM detection scheme is also called slope detection. In order for an amplitude change to be highly sensitive to the corresponding frequency change, the amplitude setpoint should be close to the position of maximum slope of the resonance curve.

In our example, we chose $\omega_{\text{drive}} < \omega_0$, corresponding to a negative force gradient (roughly: attractive tip-sample interaction). If a driving frequency larger than ω_0 is selected, this corresponds to a working point in the regime of a positive force gradient (negative negative force gradient) (roughly: repulsive tip-sample interaction).

Now we discuss the feedback process for the case of the tip scanning over a step edge as shown in Fig. 14.5c. Initially the amplitude setpoint A_1 stabilizes a frequency shift ω_1 and the corresponding tip-sample distance d_1 (working point 1 in Fig. 14.5a, b). If the tip approaches the step edge, the tip-sample distance decreases to d_2. This brings the tip into a region of larger (more negative) force gradient, shifting the resonance frequency by $\delta\omega$ to ω_2 (working point 2 in Fig. 14.5). This shift of the resonance frequency by $\delta\omega$ leads to an increase of the amplitude by δA to A_2 at ω_{drive}, as shown in Fig. 14.5b. The feedback acts on this deviation from the setpoint value A_1 by increasing the tip-sample distance d until the setpoint amplitude A_1 is restored to d_1.

In summary, a certain amplitude change corresponds to a certain resonance frequency shift, which corresponds to a certain tip-sample force gradient, which corresponds to a certain tip-sample distance $A(\Delta\omega(F'_{ts}(d)))$. Therefore, keeping the feedback loop at a constant oscillation amplitude corresponds to establishing a constant tip-sample distance. An image scanned at constant tip-sample distance is called the topography. However, this assignment is only true if the *same* frequency shift-distance relation (Fig. 14.5a) is present all over the surface.

Let us now consider scanning over a border with two different dependences of the frequency shift as a function of tip-sample distance as shown in Fig. 14.6. This will lead to an apparent height contrast even if the actual height of the atoms in both areas is the same. Initially the tip is in region A with the corresponding force gradient dependence shown in Fig. 14.6b. The setpoint frequency ω_1 stabilizes the tip-sample distance to d_A (working point 1). If by lateral scanning the tip crosses

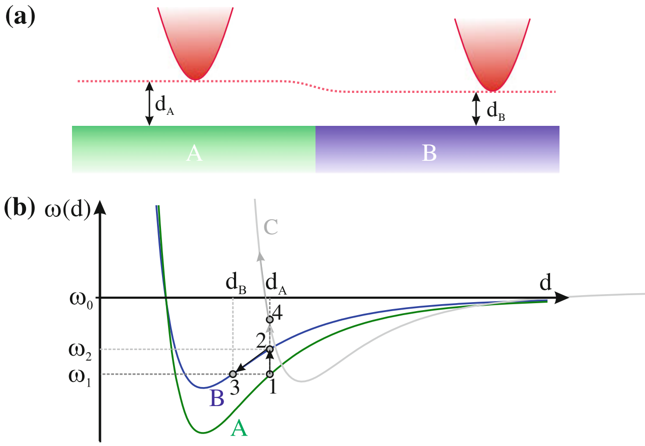

Fig. 14.6 **a** A scan from a region with material A to a region with material B can lead to a different apparent tip height in atomic force microscopy. **b** This arises due to the different force gradient-distance curves present in the two regions. For another force gradient-distance curve *C* an instability will occur due to the different sign of the slope of the force gradient, i.e. due to the non-monotonous character of the force gradient on the tip-sample distance

the border from A to B, the force gradient curve B in Fig. 14.6b applies, resulting in a different frequency shift ω_2 (working point 2). The feedback restores the setpoint frequency ω_1 by reducing the tip-sample distance to d_B (working point 3). This leads to a reduced apparent height d_B as shown in Fig. 14.6a. It is similar to the electronic effects in scanning tunneling microscopy.

While the assumed force gradient curve B resulted in a different apparent height in region B, more severe cases are also possible. Let us now assume the extreme case of the force gradient curve C in Fig. 14.6b. This case will lead to a jump to the working point 4 when the tip enters region C. At this working point the force gradient-distance curve has a negative slope and thus the feedback works in the wrong direction: The feedback will reduce the tip-sample distance in order try to restore the larger (more negative) frequency shift setpoint. While this direction of feedback was the right one for a positive slope of the force gradient curve, it is the wrong feedback direction for the opposite slope at working point 4. The feedback will constantly reduce the tip-sample distance, leading to a tip crash. This shows that the non-monotonous dependence of the force gradient on the distance can lead to serious instabilities.

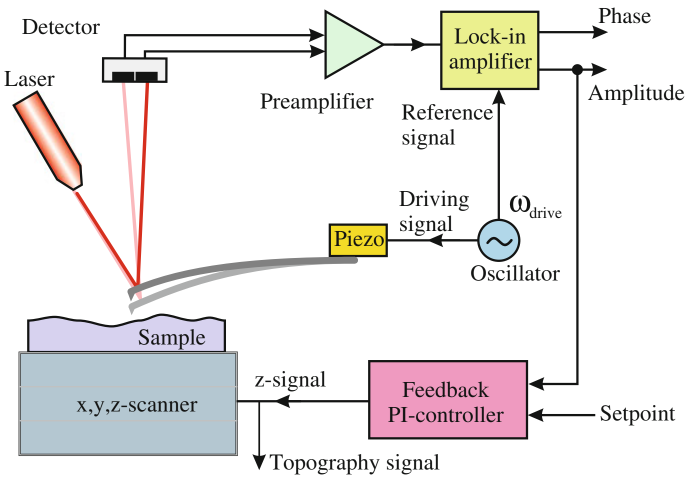

Fig. 14.7 Experimental setup for the AM detection scheme using a lock-in amplifier to detect the deviation of the oscillation amplitude from the setpoint value

14.4 Experimental Realization of the AM Detection Mode

A scheme of the experimental setup for the amplitude modulation AFM detection is shown in Fig. 14.7. The sinusoidal driving signal at ω_{drive} is generated by an oscillator. This signal excites the piezoelectric actuator driving the cantilever base.

Cantilevers have resonance frequencies of up to several hundred kHz. In order to excite such cantilevers close to their resonance frequency the piezoelectric actuator must have an even higher resonance frequency. Often this cannot be realized using a tube piezo element, since this has too low resonance frequencies. Therefore, an additional piezo plate with a high resonance frequency is used to oscillate the cantilever base and is frequently called the dither piezo element. The cantilever excitation results in a cantilever oscillation of amplitude A, which is, since it is close to resonance, much larger than the excitation amplitude. If tip and sample approach each other, the oscillation amplitude at the fixed excitation frequency ω_{drive} will change due to a shift of the resonance frequency induced by the tip-sample interaction, as discussed in the previous section. The cantilever deflection (sinusoidal signal) is measured, for instance, by the beam deflection method as indicated in Fig. 14.7. The signal from the split photodiode is converted by the preamplifer electronics to a voltage signal proportional to the cantilever deflection. This signal is an AC signal at the frequency ω_{drive} with an amplitude proportional to the cantilever oscillation amplitude A.

Using a lock-in amplifier (described in Chap. 6), the amplitude of the AC signal at frequency ω_{drive} is measured. The lock-in amplifier needs the driving signal as a reference signal. At the output of the lock-in amplifier, a quasi-DC signal of the amplitude is obtained.[4]

This quasi-DC amplitude signal (demodulated from the AC signal at $\omega_{\rm drive}$) is used as the input signal for the z-feedback controller. The measured cantilever amplitude is compared to the setpoint amplitude. The controller determines an appropriate z-signal need to maintain a constant oscillation amplitude. Via the quite indirect relation between oscillation amplitude and tip-sample distance, maintaining a constant oscillation amplitude corresponds to maintaining a constant tip-sample distance. Thus the z-feedback signal is used as the height signal, mapping the topography during data acquisition.

In the following, we describe the operation of the feedback in more detail by considering the example of a scan over a step edge. As a starting condition, we assume that before scanning over a step edge the amplitude is nicely kept closely to the amplitude setpoint value. When the step is approached laterally, the tip-sample distance will decrease. This leads, as discussed in the last section, to a deviation of the oscillation amplitude (from the setpoint amplitude) which is measured at the output of the lock-in amplifier. Thus this quasi-DC amplitude signal contains the deviations from the setpoint amplitude (e.g. due to the topography of the surface) before they are compensated by the feedback. Subsequently, this measured amplitude enters the feedback controller and deviations from the setpoint are compensated by changing the z-signal to a value equivalent to the step height. After this, the setpoint oscillation amplitude (corresponding to a certain tip-sample distance) is recovered.

A lock-in amplifier can also provide a phase signal, the difference between the phase of the cantilever oscillation and the phase of the driving signal. During a scan of the surface structure the phase signal can be recorded as free signal (i.e. not used for the feedback). This phase signal contains useful information on the tip-sample interaction, as we will discuss later in Chap. 15. Less frequently, the phase signal is used as a feedback signal and the oscillation amplitude is recorded as a free signal.

The setup shown in Fig. 14.7 can also be used to record the resonance curve of the free cantilever not in contact with the sample. This is done by disabling the feedback and ramping the driving frequency over the resonance frequency, while measuring the oscillation amplitude and the phase. The measurement of the resonance curve allows parameters like the resonance frequency ω_0, the Q-factor, and the amplitude at the resonance frequency $A(\omega_0) = A_{\rm free}$ to be determined. The value of ω_0 is needed to chose the driving frequency and $A_{\rm free}$ is needed to choose a proper amplitude setpoint.

A certain minimal detectable amplitude change in AM detection translates via the slope of the resonance curve to a minimal detectable frequency shift and finally to the resolution obtained for the tip-sample distance. The larger the slope of the resonance curve, the smaller the frequency shifts that can be detected for a given

[4] Technically the driving signal can be considered as a carrier signal which is modulated by a low-frequency (quasi-DC) amplitude signal (deviations from the desired amplitude setpoint). Then the task of the lock-in amplifier is the demodulation of the low frequency amplitude signal. The term demodulation is traditionally used in connection with signal detection in AM radio receivers. This is the reason why the term AM detection is used for this detection scheme.

minimal detectable amplitude change. The slope of the resonance curve increases with increasing Q-factor. Thus, in AM detection the sensitivity with which a frequency shift can be detected increases for higher Q-factors. However, as we will see in the following section, high Q-factors lead in the AM detection scheme to unacceptably long time constants (low bandwith). Due to this the AM detection scheme is not used for cantilevers with Q-factors larger than about 500.

14.5 Time Constant in AM Detection

The time constant for AM detection can be obtained by analyzing the solution of the equation of motion for the driven damped harmonic oscillator (2.17). The change of the motion $z(t)$ in reaction to a changed tip-sample interaction can be modeled by an (instantaneous) change of the resonance frequency of the harmonic oscillator from ω_0 to ω_0'. Either a numerical solution of the equation of motion or an analytical solution can be analyzed.

According to Sect. 2.4 the analytic solution of the equation of motion of the driven damped harmonic oscillator after a change of the resonance frequency at time $t = 0$ can be written as

$$z(t > 0) = A' \cos(\omega_{\mathrm{drive}} t + \phi') + G e^{-\omega_0' t/(2Q)} \cos(\omega_{\mathrm{hom}} t + \phi). \qquad (14.10)$$

The first term corresponds to the new steady-state oscillation at the driving frequency ω_{drive} under the influence of the shifted resonance frequency ω_0'. The new steady-state amplitude A' and phase ϕ' are given by (2.25) and (2.28), respectively, replacing ω_0 by ω_0'. The second term in (14.10) corresponds to an exponentially decreasing transient. G and ϕ are determined by the initial conditions and ω_{hom} is introduced in Sect. 2.4.

In Fig. 14.8a the envelope of the cantilever deflection $z(t)$ is plotted as a function of time for a Q-factor of 100, a resonance frequency $f_0 = 150$ kHz, and an instantaneous increase of the resonance frequency by $\Delta f = f_0 - f_0' = 1319$ Hz at time zero.[5] The envelope of the cantilever deflection $z(t)$ is plotted, since a single oscillation is not visible on the time scale shown. The transient to the new steady-state amplitude is characterized by exponential behavior and a strong beat term. The new steady-state amplitude of half of the original amplitude is reached after about Q oscillations, corresponding to a time $\tau \approx Q/(f_0 \pi) = 0.2$ ms (cf. (2.36)). This time constant still allows for fast scanning speeds in AFM scanning.

In Fig. 14.8b the time dependence of the phase is shown. The phase was determined from the cantilever deflection $z(t)$ numerically simulating a lock-in detection. Similar to the amplitude, also the phase reaches its new steady-state value after a transient of about Q oscillations.

[5] This value for the frequency shift was chosen as it leads to half of the original amplitude in the steady-state.

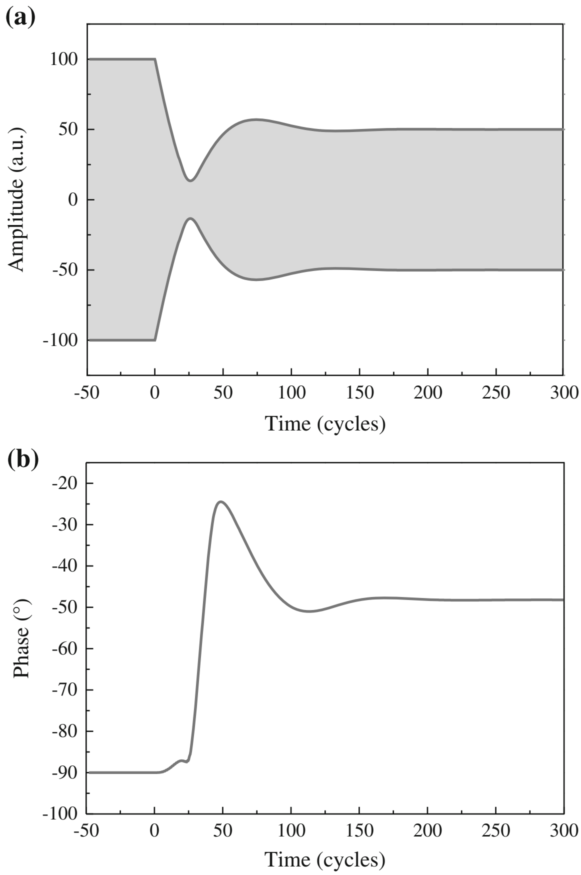

Fig. 14.8 The envelope of the oscillation amplitude (**a**) and the phase (**b**) in reaction to a change of the resonance frequency from ω_0 to ω_0' at time $t = 0$. The amplitude and phase response show that, after a transient, the new steady-state amplitude and phase are reached after about Q oscillations

For the case of a high Q-factor of 10,000, the time constant τ is 100 times larger, leading to unacceptably long scanning times when using cantilevers with a large Q-factor (i.e. in vacuum) in the AM detection mode. When the tip-sample interaction changes quickly, for instance during a fast scan over a sharp step edge, it takes several times τ before the corresponding tip oscillation amplitude changes to its new steady-state value, corresponding to the new tip-sample distance. In the transient time until the new amplitude has been established a false amplitude enters into the feedback loop, which does not yet correspond to the actual new tip-sample distance. Thus, only after this settling time can the tip be moved on to the next measuring point. For cantilevers with a high Q-factor this results in an unacceptably long scanning time. Therefore, AM detection is not used for high Q cantilevers (i.e. in vacuum). For high Q cantilevers a different detection scheme (FM detection) is used, which will be discussed in Chap. 17. The AM detection scheme is used for cantilevers under ambient conditions, where the quality factor is less than several hundred due to dissipative damping in air.

14.6 Dissipative Interactions in Non-contact AFM in the Small Amplitude Limit

Up to now we have considered the AM detection method in the limit where the tip-sample interaction is conservative. As discussed, a conservative tip-sample interaction induces a shift of the resonance frequency of the cantilever. In this section, we will consider a model which includes dissipative tip-sample interactions in a very crude way. To keep things simple, we will still deal with the small amplitude limit, i.e. an expansion of the tip-sample force up to the linear order is sufficient.

In the treatment of the simple harmonic oscillator, dissipation was included by the Q-factor. The types of dissipative forces included via the Q-factor are: energy losses (damping) if the cantilever oscillates in air or a liquid, as well as internal energy losses in the cantilever material (i.e. the cantilever itself is not 100 % elastic). This cantilever dissipation energy $E_{\text{cant}}^{\text{diss}}$ leads according to (2.41) to a corresponding Q-factor $Q_{\text{cant}} \propto 1/E_{\text{cant}}^{\text{diss}}$. An additional dissipative tip-sample interaction leads to a dissipated energy per cycle of $E_{\text{ts}}^{\text{diss}}$ and a corresponding Q-factor Q_{ts}. As the dissipation energies add up to a total dissipation energy, the inverse Q-factors add up to an effective Q-factor as

$$\frac{1}{Q_{\text{eff}}} = \frac{1}{Q_{\text{cant}}} + \frac{1}{Q_{\text{ts}}}. \tag{14.11}$$

This is not the proper way to include tip-sample dissipation, as the Q-factor takes into account only the continuous damping of the cantilever in a fluid (2.17). This damping force was considered proportional to the velocity, having its maximal value at zero amplitude of the oscillation, while the dissipative tip-sample interaction should be maximal at the lower turnaround point of the tip, i.e. closest to the sample. Nevertheless, we will now consider the damping via the effective Q-factor, since in this case we can still use the previously derived equations for the amplitude and the phase (2.25) and (2.27) of a driven damped harmonic oscillator. We use the effective quality factor and replace the resonance frequency of the free cantilever ω_0 by the shifted resonance frequency $\omega_0' = \omega_0 + \omega_0 k'/(2k)$, according to (14.6). In order to avoid too many subscripts we identify $\omega \equiv \omega_{\text{drive}}$. With this the amplitude and phase read as a function of the driving frequency ω as

$$A^2 = \frac{A_{\text{drive}}^2}{\left(1 - \frac{\omega^2}{\omega_0'^2}\right)^2 + \frac{1}{Q_{\text{eff}}^2}\frac{\omega^2}{\omega_0'^2}}. \tag{14.12}$$

and

$$\tan\phi = \frac{-\omega_0'\omega}{Q_{\text{eff}}\left(\omega_0'^2 - \omega^2\right)}, \tag{14.13}$$

respectively.

In the following, we show that in AM detection it cannot be distinguished whether a conservative interaction (leading to a frequency shift) or a dissipative interaction (leading to a different Q-factor) is the reason for a certain measured amplitude change. We consider the two limiting cases of only conservative interaction or only dissipative interaction.

In Fig. 14.9a the amplitude and phase for a free cantilever (blue curve: ω_0, Q) are compared to the case in which a conservative tip-sample interaction is included (red curve: ω_0', Q). In this case, the conservative tip-sample interaction leads to a shift of the whole resonance curve.[6] Due to the constant quality factor, the amplitude and shape of the resonance curve and phase do virtually do not change. This shift of the resonance curve and phase curve leads to a different amplitude and phase measured at the (fixed) driving frequency $\omega = \omega_{\text{drive}}$, as indicated by the vertical line in Fig. 14.9a. In this figure, the driving frequency was selected to be somewhat larger than ω_0.

The opposite assumption is that only the damping changes and the resonance frequency stays constant (ω_0, Q'). In this case, the frequency at which the maximal amplitude of the resonance curve occurs stays approximately constant very close to ω_0 with and without interaction Fig. 14.9b, while the resonance curve and the phase as a function of frequency become broader with increasing damping (lower quality factor) as shown by the green line in Fig. 14.9b. This leads to a reduced amplitude and also to a change of the phase shift at the driving frequency (vertical line in Fig. 14.9b).

As in the AM detection mode only the amplitude is measured, during scanning it is not possible to distinguish whether an amplitude change occurs due to a conservative interaction (resonance frequency shift) or due to a dissipative interaction (change of the Q-factor). Both lead to a change of the amplitude at the driving frequency. It is not known whether an initial change of A during a scan (later balanced by the feedback loop) arises due to a change of $\Delta\omega$ or Q.

The dependence of the amplitude on Q can lead to a material contrast. If in two laterally adjacent areas the true height of the two different materials as well as the conservative tip-sample interactions are the same, different damping occurring due to the two different materials can lead to a different oscillation amplitude, which results, after restoration of the amplitude by the feedback, in an apparent height difference between the two materials due to the different tip-sample dissipation.

If both A and ϕ were measured (during scanning) it is in principle possible to use these two measured values and invert (14.12) and (14.13) for ω_0' and Q_{eff}. Since (14.12) and (14.13) are a rather complicated to solve, alternatively the complete resonance curves of amplitude and phase (like the ones shown in Fig. 14.9) can be measured in a spectroscopic type of measurement. The frequency shift can then be obtained from the position of the maximum in the amplitude or the frequency at which the phase is $-90°$ so that the force gradient can be determined. The damping Q_{eff} can be determined from the width of the resonance curve in amplitude or phase.

[6] The curves in Fig. 14.9 are plotted using (14.12) and (14.13). The resonance curves for two different resonance frequencies do not exactly correspond to a shift of the resonance curve. However, Fig. 14.9a shows that these curves correspond to a very good approximation to a shift.

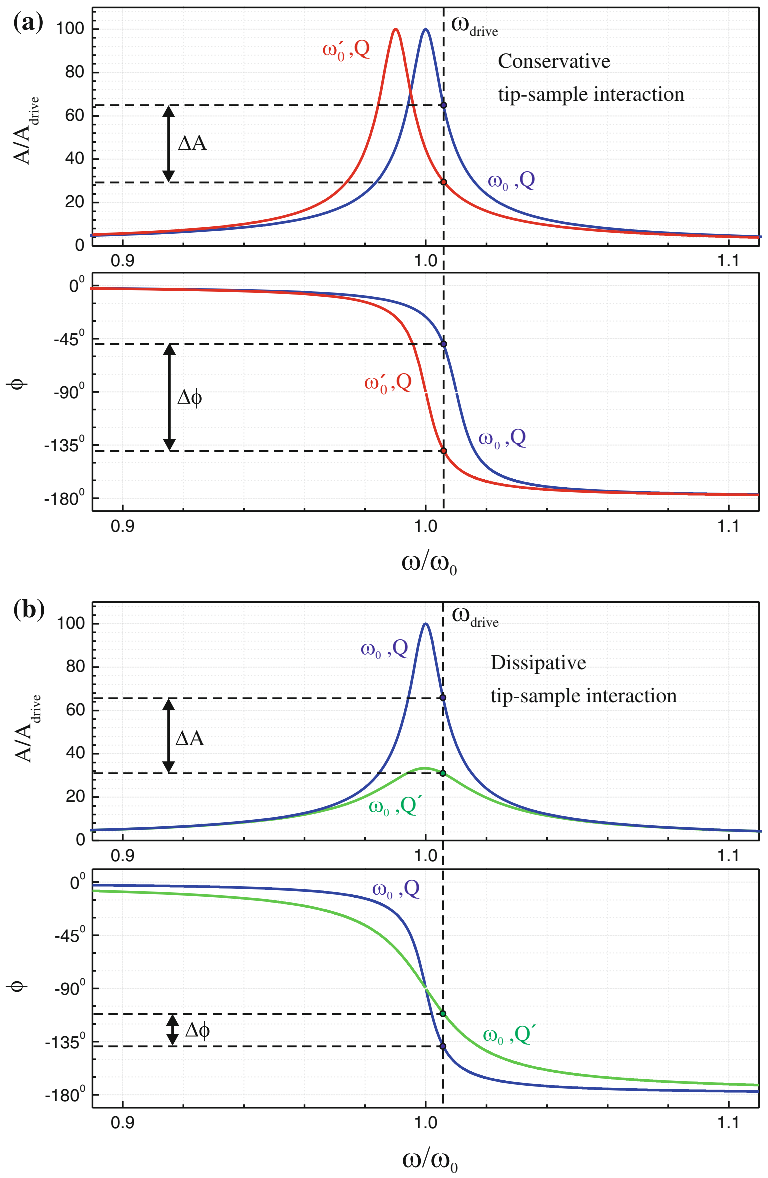

Fig. 14.9 **a** Amplitude and phase for a free cantilever (*blue curve*) compared to the case with a conservative tip-sample interaction included (*red curve*). The two resonance curves as well as the phase curves are shifted with respect to each other by $\Delta\omega$. **b** Amplitude and phase for a free cantilever compared to the case with a dissipative tip-sample interaction included (*green line*), i.e. the effective quality factor is different, while the frequency shift stays constant. In both cases (**a**) and (**b**) the oscillation amplitude at ω_{drive} is reduced, which makes it impossible to distinguish between a conservative and a dissipative interaction during scanning in the AM detection mode

All these measurements have to be performed without feedback and therefore require high stability (i.e. low drift). Further, these parameters can be obtained as a function of the tip-sample distance d at a specific location on the surface.

14.7 Dependence of the Phase on the Damping and on the Force Gradient

Generally, the dependence of the phase on the damping and on the force gradient is contained in (14.13). From Fig. 14.9, we can see that the dependence of the phase as function of frequency can be approximated as linear close to the resonance at $\omega = \omega_0$ or $\phi = -90°$. In the following, we will derive this linear relation between phase and frequency. Using in the nominator of (14.13), the approximation $\omega_0' \approx \omega_0$ and in the denominator the approximation $\omega_0' + \omega_0 \approx 2\omega_0$, as well as subsequently the relation $\Delta\omega = \omega_0' - \omega$, results in

$$\tan\phi = \frac{-\omega\omega_0'}{Q_{\text{eff}}\left(\omega_0'^2 - \omega^2\right)} \approx \frac{-\omega_0^2}{Q_{\text{eff}}\left(\omega_0' + \omega\right)\left(\omega_0' - \omega\right)} \approx \frac{\omega_0}{2Q_{\text{eff}}\Delta\omega} = \frac{k}{Q_{\text{eff}}k'}. \tag{14.14}$$

Close to the resonance, the phase will be close $-\pi/2$ and the deviation from this value will be termed the phase shift $\Delta\phi$ with $\phi = -\pi/2 + \Delta\phi$. The arctan can be approximated in this case as $\arctan x \approx -\pi/2 - 1/x$, resulting in

$$\phi = -\frac{\pi}{2} + \Delta\phi = \arctan\left(\frac{\omega_0}{2Q_{\text{eff}}\Delta\omega}\right) \approx -\frac{\pi}{2} - \frac{2Q_{\text{eff}}}{\omega_0}\Delta\omega. \tag{14.15}$$

Thus the phase shift $\Delta\phi$ relative to the phase $-90°$ results as

$$\Delta\phi = -\frac{2Q_{\text{eff}}}{\omega_0}\Delta\omega = -\frac{Q_{\text{eff}}k'}{k} = \frac{Q_{\text{eff}}}{k}\left.\frac{\partial F_{\text{ts}}}{\partial z}\right|_{z=0}. \tag{14.16}$$

This equation can be used for conversion between the frequency shift and the phase shift close to resonance. The phase shift depends linearly on both the effective quality factor and the force gradient of the tip-sample interaction. Since the phase depends on $\Delta\omega$ and Q_{eff} in a different way than the amplitude, the phase recorded as a free signal (not used for the feedback) can result in a different contrast (phase contrast) than the amplitude signal.

According to (14.16), the sign of the force gradient determines the sign of the phase shift, since Q_{eff} is always positive. For attractive forces (more precisely, positive force gradients) the phase is more negative than $-90°$ ($\phi < -90°$), and correspondingly for repulsive forces (more precisely, negative force gradients) the relation $\phi > -90°$ holds for the phase.

14.8 Summary

- If the tip oscillation amplitude is small, the tip-sample interaction can be described by a second small spring k' acting between tip and sample additionally to the cantilever spring k. The spring constant k' is given by the negative force gradient of the tip-sample interaction.
- The frequency shift of the resonance frequency under the influence of a conservative tip-sample interaction is given by

$$\Delta\omega = \omega_0 \frac{k'}{2k} = -\frac{\omega_0}{2k} \frac{\partial F_{\mathrm{ts}}}{\partial z}\bigg|_{\mathrm{z}=0}. \tag{14.17}$$

  This equation holds if the tip-sample force can be approximated as linear within the range of the oscillation amplitude and if $|k'| \ll k$.
- Roughly, the frequency shift $\Delta\omega$ is positive (towards higher frequencies) for repulsive forces and negative for attractive forces.
- In the amplitude detection mode (AM), the cantilever is driven at a fixed frequency and amplitude. The oscillation amplitude (and phase) is measured using the lock-in technique and used as the feedback signal.
- The measured oscillation amplitude depends on the frequency shift of the resonance curve induced by the tip-sample interaction. Feedback on constant oscillation amplitude corresponds to constant frequency shift and finally constant tip-sample distance.
- The non-monotonous dependence of the frequency shift on the tip-sample distance can lead to instabilities in the feedback behavior.
- A measured change of the amplitude (phase) during imaging in the AM mode can be induced by a frequency shift (conservative interaction) as well as by a change in quality factor (dissipative interaction).
- The phase shift close to the resonance is proportional to the frequency shift as $\Delta\phi = -\frac{2Q_{\mathrm{eff}}}{\omega_0}\Delta\omega$. Thus the phase shift depends linearly on Q_{eff} and the force gradient.

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