Phase shifts and energy dissipations of several modes of AFM:
Minimizing topography and dissipation measurement errors

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ABSTRACT

For clear interpretation of a sample’s surface properties, several simple and general relations between phase shifts of atomic force microscopy (AFM) and sample’s properties are derived. The topography and dissipation measurement errors due to some inherent uncertainties are investigated. For derivation of these simple and general relations among measuring signals and sample’s properties, the dynamic behavior of a cantilever is simulated into a mass-spring-damper model. In general, the conventional model can determine the first mode only. The dynamic effective spring theory is introduced here. Based on this theory, the conventional model can be modified to accurately determine the dynamic motions of higher modes of a cantilever. If the dynamic behavior is almost harmonic, the exact dynamic response of the general system subjected to arbitrary tip–sample force is derived. Moreover, several simple and general relations among dynamic responses of AFM and sample’s properties are discovered. Based on these relations, the errors of measuring a sample’s surface properties due to the inherent measuring uncertainties are investigated. Finally, some methods to minimize the error of measurement are proposed.

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1. Introduction

Atomic force microscopy (AFM) has been widely developed as a powerful technique for obtaining atomic-scale images and the material surface properties [1–2]. For example, AFM is used to image DNA, proteins and polymers in air or liquids [2] and for precision metrology [3]. When a soft sample such as DNA, protein and polymer is imaged, there exists a damping force between a cantilever tip and a sample [4–17]. For studying the morphologies and nanostructures of samples, the energy dissipation, the frequency shift and the phase angle of an AFM subjected to a damping force must be investigated. Moreover, if some simple and general relations among these measured parameters and a sample’s topography and properties are obtained, it will improve greatly the studies of a sample’s surface topography and properties. Unfortunately, so far, no simple and general relation is discovered yet.

In general, dynamic behavior of an AFM is simulated by using the beam theory [11,13,14,18–22] and the effective spring-mass-damper model [5–12,15–17,23]. The elementary beam theory is commonly known as the Euler–Bernoulli beam theory. The mathematical equations based on the beam theory are too complex to derive a simple and general relation among the tip response and a sample’s surface properties. For simplicity, the cantilever is usually approximated by an effective spring-mass-damper model. The equation of motion of a spring-mass-damper model is an ordinary differential equation which is easily solved. However, because an effective spring-mass-damper model has one degree of freedom, only the first mode can be commonly derived. So far, it is well known that measuring the response of higher modes is helpful for studying a sample’s properties. For example, Sommerhalter et al. [24] and Glatzel et al. [25] proposed that the first resonant frequency was used to measure the sample’s topography and the second resonant frequency for the potential measurement.

The principle of dynamic force microscopy is to measure the tip–sample force for studying a sample’s surface topography and properties. There are many kinds of tip–sample forces such as the van der Waals one, the electrostatic force, and the damping force, etc. The electrostatic force includes both one due to the tip–sample potential difference and another one due to artificial ac and dc bias voltage between tip and sample [26]. Sadewasser et al. [27,28] investigated the resolution of Kelvin probe force microscopy (KPFM) and the influence of uncompensated electrostatic force on a sample’s surface height measurements. KPFM is a scanned probe method where the potential offset between a probe tip and a surface can be measured. The cantilever in the AFM is a reference electrode that forms a capacitor with the surface, over which it is scanned laterally at a constant separation. The cantilever is not
piezoelectrically driven at its mechanical resonance frequency \( \omega_0 \) as in normal AFM although an alternating current (ac) voltage is applied at this frequency. Sadewasser et al. found that the measured step height was strongly dependent on the dc bias voltage between tip and sample. However, there is no accurate and general discussion about the phenomenon yet. Moreover, Tamayo and Garcia [29], Cleveland et al. [30] and Wang et al. [31] investigated the relation between the phase shift of the first mode and the energy dissipation. This simple and approximated relation is derived and listed in Eqs. (31a) and (31b). It is suitable only for the system with small damping. Moreover, to determine the phase shift the tip amplitudes of a cantilever with and without a tip–sample force must be measured. The details are discussed in Section 3.

In this study, the complete effective energy theory will be introduced to improve the proposed method given by Lin [32], which is successfully used to derive the exact dynamic response of the first mode of a mass-spring-damper system subjected to the van der Waals force. Then this mass-spring-damper model can be used to simulate the dynamic motion of higher modes subjected to arbitrary tip–sample force. Several exact relations among a sample’s properties and tip responses are derived. Based on these relations, the effects of an inherent uncertainty of measurement and a compensated dc bias voltage on the topography and sample’s properties measurement errors are also investigated. Moreover, a methodology to minimize measurement errors is proposed.

2. Effective energy theory and dynamic response of several modes

For simplicity, the dynamic force microscopy is usually simulated by a mass-spring-damper system as shown in Fig. 1. However, it is usually used to study the dynamic behavior of the fundamental mode only. This disadvantage has been overcome by Lin et al. [33] by using the dynamic effective spring constant to improve a conventional perturbation method to determine the resonant frequency shifts of higher modes. However, the dynamic behaviors of higher modes have not been discussed yet. In this study, the complete effective energy theory is introduced to simulate the dynamic motion of the ith mode of a mass-spring-damper model. The assumptions of this theory are as follows:

1. The spring strain energy of the effective mass-spring-damper model is equal to a cantilever’s strain energy of the ith mode.
2. The spring deformation of the effective model is equal to the tip amplitude of a cantilever.
3. The ith mode natural frequency of the effective model is equal to that of a cantilever.

According to these assumptions, one can derive the ith mode effective spring constant \( k_i \) called as a dynamic effective spring constant. Further, the ith effective mass is \( m_i = k_i/[(2\pi f_i)^2] \) where \( f_i \) is the ith natural frequency of a cantilever. The ith mode mathematical equation of motion is expressed as

\[
m_i \ddot{z} + c_i \dot{z} + k_i z(t) = F_{ts} + g_i k_i (t - t_{0,i})
\]

where the subscript ‘i’ denotes the ith mode, \( z \) represents the tip displacement, \( k_i \) and \( m_i \) are the dynamic effective spring constant and the effective mass, respectively. \( c_i \) is the total damping coefficient which includes both the free vibration damping one \( c_0 \) and the tip–sample damping one \( c_{ts} \) [10]. \( F_{ts} \) is the tip–sample force. \( g_i \) is the gain factor which is the amplification factor of the displacement signal in the closed-loop control system. The base displacement is \( g_i z(t - t_{0,i}) \) where \( t_{0,i} \) is the ith mode time difference between the responses of the tip and the base of beam. \( 1/g_i \) represents the response ratio of the amplitude of tip to that of base excitation.

If the dynamic response is almost harmonic, the solution of Eq. (1) can be expressed as

\[
z(t) = A \cos(2\pi ft)
\]

where \( A \) is the tip amplitude and \( f \) a frequency of the base excitation. Substituting the solution into Eq. (1), multiplying it by \( \cos(2\pi ft) \) and integrating it from 0 to the period \( T_i, 2\pi f_i / \Omega_i \), one obtains

\[
g_i \cos 2\pi f_{ts,0,i} = -s_i^2 + 1 - \frac{1}{\pi k_i A} \int_0^{2\pi} F_{ts} \cos \chi \, d\chi
\]

where \( s_i = s_{f0,i} \) and \( F_{ts} = F_{ts}(D_0 - A \cos \chi) \) in which \( D_0 \) is the distance between the tip of the undeformed beam and the surface of sample, \( f_{0,i} \) the ith natural frequency of the cantilever not subjected to the tip–sample force and \( \chi = 2\pi ft \). Similarly, substituting Eq. (2) into Eq. (1), multiplying by \( \sin(2\pi ft) \) and integrating it from 0 to the period \( T, 2\pi / \Omega \), one obtains

\[
g_i \sin 2\pi f_{ts,0,i} = -2\gamma_i s_i - \frac{1}{\pi k_i A} \int_0^{2\pi} F_{ts} \sin \chi \, d\chi
\]

where the total damping ratio \( \gamma_i = \gamma_{0,i} + \gamma_{ts,i} \) in which \( \gamma_{0,i} = \pi f_{0,i} c_0 / k_i \) and \( \gamma_{ts,i} = \pi f_{ts,i} c_{ts} / k_i \). Dividing Eq. (4) by Eq. (3), the ith mode phase angle \( \phi_i \) is obtained

\[
\tan \phi_i = \frac{2\gamma_i s_i + (1/\pi k_i A) \int_0^{2\pi} F_{ts} \sin \chi \, d\chi}{s_i^2 - 1 + (1/\pi k_i A) \int_0^{2\pi} F_{ts} \cos \chi \, d\chi}
\]

where \( \phi_i = 2\pi f_{ts,0,i} \). Taking the square of (3) and (4) and summing these, the amplitude ratio is obtained

\[
g_i^2 = \left[ -s_i^2 + 1 - \frac{1}{\pi k_i A} \int_0^{2\pi} F_{ts} \cos \chi \, d\chi \right]^2
\]

\[
+ \left[ -2\gamma_i s_i - \frac{1}{\pi k_i A} \int_0^{2\pi} F_{ts} \sin \chi \, d\chi \right]^2
\]

Obviously, the amplitude ratio depends on the tip–sample force \( F_{ts} \), the dynamic effective spring constant \( k_i \) and the damping ratio \( \gamma_i \), the frequency ratio of excitation \( s_i \) and the tip amplitude \( A \). Both the phase angle \( \phi \) and the amplitude ratio \( g \) greatly depend on the frequency ratio \( s_i \). It is well known that if the base amplitude \( A_{\text{base}} \) is fixed, the tip amplitude \( A \) is the maximum at the resonance. In other words, if the tip amplitude \( A \) is fixed, the amplitude of the exciting root, \( A_{\text{base}} = gA \), is the minimum at the resonance. According to the condition, one can derives the following relation among the resonant frequency ratio, the tip–sample force, and other
parameters
\[ s_{res,i}^3 = \left[-1 + 2\gamma_{t,i}^2 + \frac{1}{\pi k a} \int_0^{2\pi} F_s \cos \chi \, d\chi \right] s_{res,i} \]
\[ - \frac{\gamma_{t,i}}{\pi k a} \int_0^{2\pi} F_s \sin \chi \, d\chi = 0 \]  \hspace{1cm} (7)

Because \( D = D_0 - z(t) = D_0 - A \cos \omega t \) which is an even function, \( F_{ts}(D) \) is also even. It results in that \( \int_0^{2\pi} F_s \sin \chi \, d\chi = 0 \). Therefore, Eq. (7) becomes
\[ s_{res,i} = \sqrt{1 - 2\gamma_{t,i}^2 - \frac{1}{\pi k a} \int_0^{2\pi} F_s \cos \chi \, d\chi} \]  \hspace{1cm} (8)

It should be noted that \( F_s \) is arbitrary tip–sample force.

3. Relations among dynamic responses and material’s properties

Commonly, measuring the difference between the phase angles of the tip and the base of a cantilever predicts a sample’s surface energy dissipation. The effects of the van der Waals force \( F_v \), the electrostatic force \( F_e \), and the damping force \( c_z \) on the dynamic response of AFM are investigated. The tip–sample force is expressed as
\[ F_{ts} = F_v + F_e \]  \hspace{1cm} (9)

where the van der Waals force is \([12]\)
\[ F_v = -\frac{A_{ff}R}{6D^2} \]  \hspace{1cm} (10)
in which the tip–surface distance \( D = D_0 - z(t) \), \( A_{ff} \) the Hamaker constant and \( R \) is the tip radius. The electrostatic force is expressed as \([25]\)
\[ F_e = \frac{1}{2} \frac{\partial C}{\partial z} (V_{dc} - V_{cp})^2 \]  \hspace{1cm} (11)
where \( V_{dc} \) is the contact potential difference between a probe and a sample. \( V_{dc} \) is a compensated dc voltage. \( \partial C/\partial z \) is the spatial derivative of the capacitance between a probe and a sample. The derivative of the capacitance of a tip modeled as a spherical apex and cone, is modeled by Hudlet et al. \([34]\) as follows:
\[ \frac{\partial C}{\partial z} = 2\pi \varepsilon_0 F(D) \]  \hspace{1cm} (12)
where \( \varepsilon_0 \) is the vacuum permittivity and
\[ F(D) = -K^2 \left[ \ln \left( \frac{H}{D + R(1 - \sin \theta)} \right) - 1 + \frac{R \cos \theta}{D + R(1 - \sin \theta)} \right] - \frac{R^2 D^2 (1 - \sin \theta)}{D[D + R(1 - \sin \theta)]} \]  \hspace{1cm} (13)
in which \( K = 1/[\ln(\tan(\theta/2))] \) and \( \theta \) is the half open angle of the tip. Law and Rieutord \([35]\) verified that the model (13) was very good in agreement with the experiment. One can derive the following integrals:
\[ \int_0^{2\pi} F_s \sin \chi \, d\chi = 0 \quad \text{and} \quad \int_0^{2\pi} F_s \cos \chi \, d\chi = F_{vc} + F_{ec} \]  \hspace{1cm} (14)
where
\[ F_{vc} = \int_0^{2\pi} F_v \cos \chi \, d\chi = \frac{2\pi A_{ff} R}{6(D_0^2 - A^2)^{3/2}} \]
\[ F_{ec} = \int_0^{2\pi} F_e \cos \chi \, d\chi = -2\pi^2 \varepsilon_0 (V_{dc} - V_{cp})^2 K^2 \]
\[ \times \left[ (1 - \sqrt{1 - c^2}) + \frac{a}{b_3} \left( 1 - \frac{a_3}{\sqrt{a_2^2 - b_3^2}} \right) \right] - 2\beta \left( \frac{A_1}{\sqrt{a_1^2 - b_1^2}} + \frac{A_2}{\sqrt{a_2^2 - b_2^2}} \right) \]  \hspace{1cm} (15)
in which
\[ A_1 = \frac{a_1}{(a_1 b_2 - a_2 b_1)^2}, \quad A_2 = \frac{-a_2}{(a_1 b_2 - a_2 b_1)^2}, \]
\[ a_1 = D_0, \quad b_1 = b_2 = b_3 = -A, \]
\[ a_2 = a_3 = D_0 + R(1 - \sin \theta), \quad c = b_3/a_3, \]
\[ \alpha = K \frac{\cos^2 \theta}{\sin \theta}, \quad \beta = K^2 (1 - \sin \theta). \]
The corresponding phase angle is derived
\[ \tan \phi_1 = \frac{2\gamma_{t,i} \varepsilon_0}{s_{res,i}^3 - 1 + ((F_{vc} + F_{ec})/\pi k a)} \]  \hspace{1cm} (17)

It is observed from Eq. (17) that if there is no damping force between a tip and a sample, the phase angle difference between the motions of the tip and the base of a cantilever is zero. Moreover, the corresponding resonant frequency becomes
\[ s_{res,i} = \sqrt{1 - 2\gamma_{t,i}^2 - (F_{vc} + F_{ec})/\pi k a} \]  \hspace{1cm} (18)

In general, the tip–sample force \( F_{ts} \) is much smaller than the restoring force \( k a \) and the damping coefficient is very small. In other words, \( 2F_{ts} + (F_{vc} + F_{ec})/\pi k a \ll 1 \). It results in that \( s_{res,i} \approx 1 - \gamma_{t,i}^2 (F_{vc} + F_{ec})/2\pi k a \) or the frequency shift \( \Delta f \approx -f_0 \gamma_{t,i}^2 (F_{vc} + F_{ec})/2\pi k a \). Further, if the damping ratio is zero, the frequency shifts are the same as those derived by using the perturbation method. Substituting Eq. (18) back into Eq. (6), the resonant response ratio is obtained
\[ \frac{1}{\Delta f_{res,i}} = \frac{1}{2\gamma_{t,i} \sqrt{1 - \gamma_{t,i}^2 - ((F_{vc} + F_{ec})/\pi k a)}} \]  \hspace{1cm} (19)
It should be noted that the viscous damping ratio \( \gamma_{t,i} \) can be calculated via Eq. (19) by measuring the resonant response ratio \( 1/\Delta f_{res,i} \).

In general, the Q-factor is defined as
\[ Q\text{-factor} = 2\pi \frac{E_{total}}{\Delta E_{loss,t}} \]  \hspace{1cm} (20)
where \( \Delta E_{loss,t} \) is the total energy loss per cycle
\[ \Delta E_{loss,t} = \int \left[ c_i \frac{dz(t)}{dt} \right] dz(t) = 2\pi^2 c_i A^2 f \]  \hspace{1cm} (21)
It should be noted that the total energy loss is due to both the material and environmental damping of a cantilever and the tip–sample damping. The total energy loss per cycle is expressed as \( \Delta E_{loss} = \Delta E_{loss,0} + \Delta E_{loss,ts} \) where \( \Delta E_{loss,0} = 2\pi^2 c_i A^2 f \) and \( \Delta E_{loss,ts} = 2\pi^2 c_i A^2 f \). For interpretation of a sample surface’s properties, the energy loss due to the tip–sample damping is greatly
concerned. $E_{\text{total}}$ is the total average energy which is usually approximated by the maximum strain energy

$$E_{\text{total}} = \frac{1}{2} k_i A^2$$

(22)

Substituting Eqs. (21) and (22) back into Eq. (20), the Q-factor is obtained

$$Q = \frac{1}{2} \gamma_i s_i$$

(23)

where the damping ratio $\gamma_i = \frac{D_{\text{loss},s}/2\pi A^2 kr}{D_{\text{loss},0}}$. Without the tip–sample interaction, the Q-factor of a cantilever is $Q_0 = 2\pi E_{\text{total}}/D_{\text{loss},0}$. Substituting it back into Eq. (20), the influence of the tip–sample energy dissipation on the Q-factor can be obtained

$$\Delta E_{\text{loss},ts} = \Delta E_{\text{loss},0} \left( \frac{Q_0}{Q} - 1 \right)$$

(24)

It is the same as that given by Morita et al. [36]. In particular, the Q-factor is usually defined at the resonant frequency even at that without a tip–sample force. However, the resonant frequency depends on the tip–surface force. For clarity and generality, Eq. (20) is proposed for any measuring case with arbitrary frequency of excitation. Substituting the resonant frequency (18) into Eq. (23), the Q-factor of the ith mode subjected to the tip–sample forces, is

$$Q_{\text{res},i} = \frac{1}{2\gamma_i \sqrt{1 - 2\gamma_i^2 - \left( (F_{\text{res}} + F_{\text{ec}})/\pi k_i A \right)}}$$

(25)

It is found that if the van der Waals force and the electrostatic force and the damping are very small, $Q_{\text{res},i} \approx 1/\gamma_i \approx 1/2\gamma_i$. Moreover, if the tip–sample forces are neglected and the damping is small, the resonant Q-factor becomes $Q_{\text{res},i} \approx 1/\gamma_i = k_i/q_0 \omega_0$ which is well known in a discrete system without the tip–sample interaction [37].

Substituting Eq. (14) into Eq. (17), the relation between the phase angle and the energy dissipation is derived

$$\tan \phi_i = \frac{\Delta E_{\text{loss},0} + \Delta E_{\text{loss},ts}}{\pi A^2 k_i (s_i^2 - 1) + (F_{\text{res}} + F_{\text{ec}})/\pi k_i A]}$$

(26)

In the neglect of a tip–sample force, Eq. (26) becomes $\tan \phi_0,i = \Delta E_{\text{loss},0}/\pi A^2 k_i (s_i^2 - 1)$ where $\phi_0,i$ is the phase angle without the tip–sample interaction. Further, Eq. (26) can be expressed as

$$\tan \phi_i = \frac{\Delta E_{\text{loss},ts}}{\pi A^2 k_i (s_i^2 - 1) + (F_{\text{res}} + F_{\text{ec}})/\pi k_i A]}$$

$$+ \frac{(s_i^2 - 1)}{[s_i^2 - 1 + (F_{\text{res}} + F_{\text{ec}})/\pi k_i A]} \tan \phi_0,i$$

(27)

This is simple and helpful for interpreting a sample’s surface property by measuring the phase change of a cantilever. It is observed from Eq. (27) that if the phase angle is used to measure the tip–sample energy dissipation, decreasing the amplitude $A$ and the spring constant $k_i$ will increase the ratio $\tan \phi_i/\Delta E_{\text{loss,ts}}$. In other words, these will increase the sensitivity of determining the energy loss $\Delta E_{\text{loss,ts}}$. Moreover, the sensitivity by using the first mode is larger than that by using the higher mode. Intuitively, determining the energy dissipation by using the first mode is optimum. However, in addition to the energy dissipation, the phase shift also depends on other parameters. The complete discussion will be made in Section 4.2. Moreover, if $s_i \approx 1$, Eq. (27) becomes $\tan \phi_i \approx \Delta E_{\text{loss,ts}}/A(F_{\text{res}} + F_{\text{ec}})$. Because the interacting forces ($F_{\text{res}}$, $F_{\text{ec}}$) depend greatly on the tip–sample distance, the influence of the step height of a sample’s surface on the phase angle becomes significant. The error of measuring a sample’s topography will result in a large error of measuring the energy loss per cycle.

Conventionally, based on the conservation of energy, one can also derive another relation between the phase angle and the energy dissipation. When a cantilever is excited at its root by the value of $z_{\text{base}}(t)$, there is an energy per cycle imported from the root $\Delta E_{\text{input}}$. However, there are two ways of dissipating the input energy $\Delta E_{\text{input}}$: (1) the basic energy dissipation $\Delta E_{\text{loss},0}$ due to the material damping of the cantilever and the air damping, and (2) the energy dissipation $\Delta E_{\text{loss},ts}$ due to the interaction between the tip and the sample’s surface. In practice, the cantilever without the tip–sample force is excited at its root by the value of $z_{\text{base}}(t)$, the basic energy dissipation $\Delta E_{\text{loss},0}$ and the resonant Q-factor $Q_0,\text{res}$ can be measured. Based on the conservative principle of energy, it is expressed as

$$\Delta E_{\text{loss},ts} = \Delta E_{\text{input}} - \Delta E_{\text{loss},0}$$

(28)

where

$$\Delta E_{\text{input}} = \int_0^T F_{\text{base}} dt = \pi k_0 A^2 \sin \phi$$

(29)

in which the base force $F_{\text{base}} = k_0 z(t) - z_{\text{base}}(t)$ and the base displacement $z_{\text{base}}(t) = g(t - t_0)$. Substituting Eq. (29) and $\Delta E_{\text{loss},0}$ into Eq. (28), one obtains

$$\Delta E_{\text{loss},ts} = \pi A^2 (k_0 \sin \phi - c_0 \omega)$$

(30)

If the damping is very small, $Q_0,\text{res} \approx k_0/c_0 \omega_0$ and Eq. (30) can be written as

$$\sin \phi = \frac{\omega}{\omega_0} + \frac{\Delta E_{\text{loss},ts}}{\pi A^2 k_0} = \frac{A_0}{(Q_0,\text{res}(Ag)) \omega_0} + \frac{Q_0,\text{res} \Delta E_{\text{loss},ts}}{\pi A k_0}$$

(31a)

Because $Ag = A_{\text{base}}$ and $A_0 = Q_0,\text{res} A_{\text{base}}$ where $A_0$ is the tip amplitude of a cantilever not subjected to a tip–sample force, Eq. (31a) can be expressed as

$$\sin \phi = \frac{\omega A_0}{\omega_0 A_0} + \frac{Q_0,\text{res} \Delta E_{\text{loss},ts}}{\pi A_0}$$

(31b)

which is the same as that given by Tamayo and Garcia [29]. But there exists some disadvantage of Eq. (31b) discussed as following. Based on the above statements of its derivation, it is necessary to measure the tip amplitudes $A$ and $A_0$ under the same root excitation $z_{\text{base}}(t)$. In other words, one needs to firstly measure the tip amplitude $A_0$ of the cantilever without the tip–sample force and then measure the tip amplitude $A$ of the cantilever subjected to the tip–sample force. These measurements must be under the same root excitation $z_{\text{base}}(t)$. In other words, two signals of measuring the tip and root amplitudes $A$ and $A_{\text{base}}$ must be recorded simultaneously. This way is more complex than that via Eq. (27) which only the tip amplitude $A$ is needed. Further, if the frequency of excitation approaches the resonant frequency, $A_{\text{base}}$ is too small to be measured accurately. In the summary, the measuring methodology via Eq. (27) is more accurate and simple than that via the conventional relations (31a) and (31b).

4. Topography and dissipation measurement errors

Based on these relations derived above, one can predict the errors of measuring a sample’s surface topography and properties due to inherent parameters’ tolerances.
4.1. Error of measuring a sample’s topography

Sadewasser et al. [28] investigated the influence of uncompensated electrostatic force on height measurement in non-contact AFM. They found that the measured step height $\Delta z_{\text{mea}}$ clearly depended on the dc bias voltage. A correct height measurement was possible only if two different contact potential values were known and the optimized compensation dc voltage was applied. Lin [32] found that increasing the tip radius $R$ and the damping ratio $\gamma$ increases the error of measuring a sample’s surface topography without the effect of electrostatic force. In this study, the effect of a compensated dc voltage on the error of measuring a sample’s topography is investigated. The error of height measurement in non-contact AFM due to uncompensated electrostatic force can be derived by using Eq. (18). Commonly, a nano–wire is coated on a substrate. Their contact potential differences are different and denoted as $\{V_{cp,a}, V_{cp,b}\}$, as shown in Fig. 2. If no compensated dc voltage is given and $V_{cp,a} = 0$, the electrostatic force at position ‘a’ $F_{ec,a} = 0$ and Eq. (18) can be expressed as

$$F_{ec,a} = 4\pi^3 m_A (f_0^2 - 2)^2 f_0^2 (f_1, f_0^2 - f_{res,i})$$

(32)

Further, during measuring the height of position ‘b’, if a correct compensated dc bias voltage is given, i.e., $V_{dc} = V_{cp,b}$ and $F_{ec,b} = 0$, the height difference, called as step height, between two surface positions ‘a’ and ‘b’ is to be measured exactly. For a perfect measurement, whenever any point of a sample’s surface is measured, the amplitude, the resonant frequency and the damping ratio must be kept to be constant. If these conditions are kept, $F_{ec,b} = F_{ec,a}$ and the height of the piezoelectric scanning table must be adjusted so that the tip–sample distances are the same while measuring the two surface points ‘a’ and ‘b’, $D_{0,b} = D_{0,a}$. The adjusted step height $\Delta h_{\text{mea}}$ is the real height $\Delta h_{ab}$ between the two points. Unfortunately, if $V_{dc} \neq V_{cp,b}$, then $F_{ec,b} \neq 0$ and $\Delta h_{\text{mea}} \neq \Delta h_{ab}$. It is obvious that decreasing the electrostatic force $F_{ec,b}$ will decrease the error of measuring the step height. According to this requirement, it is proposed via Eq. (15) that decreasing the tip radius and the cone angle of tip decreases the electrostatic force $F_{ec,b}$. It is concluded that decreasing the tip radius and the cone angle of tip decreases the error of measuring a step height of a sample’s surface due to an unsuitable compensation of dc bias voltage.

Fig. 2(a) shows the relationship among the first frequency shift, the measured step height $\Delta z_{\text{mea}}$, and the dc bias voltage $V_{dc}$. It is found that if $\Delta f_1 = -20$ Hz, an inaccurate compensation of dc voltage results in a large error of a measured step height. But increasing the first frequency shift greatly decreases the error due to the compensation of dc voltage. It should be noted that decreasing the distance between the tip of the undeformed beam and the surface of sample, $D_0$, increases the frequency shift [18]. In a similar way, the influence of the tip radius on the error of measuring a
4.2. Error of measuring the energy dissipation

The complete relation between the phase angles and a sample’s surface energy loss per cycle has been derived above. In reality, there must be the inherent tolerances of the tip amplitude, the phase angle, a step height, the frequency of excitation and electrostatic force. These parameters will result in an error of measuring the energy dissipation. Thus their effects on the error are investigated here. Eq. (27) is also expressed as

$$\Delta E_{\text{loss},ts} = \pi \alpha^2 k_{\text{i}} \left\{ \left( \frac{s_i^2}{2} - 1 + \frac{1}{\pi k_{\text{i}} A} \int_0^{2\pi} F_T \cos \chi d\chi \right) \times \tan \phi_i - (s_i^2 - 1) \tan \phi_{0,i} \right\} \quad (33)$$

According to Eq. (33), if the tip–sample force $F_T$ is much smaller than the restoring force $k_{\text{i}} A$ or $\int_0^{2\pi} F_T \cos \chi d\chi / \pi k_{\text{i}} A \ll (s_i^2 - 1)$, the error of the measured energy loss per cycle only due to the error of the tip amplitude $\Delta A$ is derived

$$\text{error}_{\text{loss},ts} \approx \pi k_{\text{i}} (s_i^2 - 1) \left( \tan \phi_i - \tan \phi_{0,i} \right) \left\{ 2A \Delta A + \Delta A^2 \right\} \quad (34a)$$

It is observed from Eq. (34a) that increasing the amplitudes of oscillation and the effective spring constant increases significantly the error of measuring energy loss per cycle. Further, if $\int_0^{2\pi} F_T \cos \chi d\chi / \pi k_{\text{i}} A \ll (s_i^2 - 1)$ and $s_i \rightarrow 1$, the error of measuring energy loss per cycle will be decreased. However, only if $s_i \rightarrow 1$, the error of the measured energy loss per cycle only due to the error of the tip amplitude $\Delta A$ becomes

$$\text{error}_{\text{loss},ts} \approx \pi A \tan \phi_i \int_0^{2\pi} F_T \cos \chi d\chi \quad (34b)$$

It is observed from Eq. (34b) that the error of measuring a sample’s topography will result in a large error of measuring the energy loss per cycle. Similarly, if the tip–sample force $F_T$ is much smaller than the restoring force $k_{\text{i}} A$ or $\int_0^{2\pi} F_T \cos \chi d\chi / \pi k_{\text{i}} A \ll (s_i^2 - 1)$, the error of the measured energy loss per cycle only due to the error of the frequency of excitation is derived

$$\text{error}_{\text{loss},ts,s} \approx \pi k_{\text{i}} A^2 \left( \tan \phi_i - \tan \phi_{0,i} \right) \left\{ 2 \Delta A \delta_s + \Delta s_i^2 \right\} \quad (35)$$

Because the frequency is very large and easily controlled, $\Delta s_i$ is usually very small. Therefore, the topography error due to the frequency excitation error should be neglected.

Fig. 3 shows the influence of the first two frequency shifts ($\Delta f_1$, $\Delta f_2$), the energy loss per cycle $\Delta E_{\text{loss},ts}$, the compensated dc voltage $V_{\text{dc}}$ and the tip–sample distance $D_0$ on the phase angle $\phi$. Fig. 3(a) and (b) are for the first two modes, respectively. Fig. 3(a) shows that when the excitation frequency $f$ approaches the first natural frequency $f_1$, i.e., $s_1 \rightarrow f_1 - 1$ or $\Delta f_1 = f - f_1 \rightarrow 0$, although the energy loss per cycle is constant, the phase angle changes greatly with the compensated dc voltage and the tip–sample distance. In other words, if the compensated dc voltage and the tip–sample distance are not correctly applied, the energy dissipation cannot be accurately calculated by using the measured phase angle. But if the first frequency shift is increased and the energy loss per cycle is constant, the phase angle changes slightly with the compensated dc voltage and the tip–sample distance. It means that if the first frequency shift $\Delta f_1$ is increased, although the compensated dc voltage and the tip–sample distance are not correctly applied, the energy dissipation can be accurately calculated by using the measured phase angle.

Fig. 3(b) shows that if the second frequency shift $\Delta f_2 = -80$ Hz and the energy dissipation $\Delta E_{\text{loss},ts} \approx 2.43$ or 15.26 eV, the phase angle $\phi_2$ of the second mode is almost independent of the compensated dc voltage and the tip–sample distance. Moreover, the relation between $\phi_2$ and $\Delta E_{\text{loss},ts}$ is one to one. It means that if $\Delta f_2 = -80$ Hz, no matter what the compensated dc voltage and the tip–sample distance are, one can get an accurate energy dissipation by measuring the phase angle of the second mode. But when the second frequency shift $\Delta f_2$ is decreased, the phase angle greatly depends on the compensated dc voltage $V_{\text{dc}}$ and the tip–sample distance $D_0$. It means that if the second frequency shift $\Delta f_2$ is small, it is difficult to accurately determine the energy dissipation by measur-
ing the second phase angle unless $\left( V_{dc}, A_0 \right)$ are correctly applied. Moreover, it is observed from Fig. 3(a) and (b) that the influence of the tip–sample distance and the dc voltage on the second phase angle is weaker than that of the first mode. In summary, it is better to use the phase angle of the second mode to calculate the energy dissipation than to use the phase angle of the first mode. It is the reason that if a large frequency shift is considered, one can get a one to one relation between the phase shift and the energy dissipation. Although the compensated dc voltage and the tip–sample distance are not correctly applied, the accurate energy dissipation can be determined by measuring the phase angle of the second mode.

5. Conclusions

The dynamic measurement of an atomic force microscopy is simulated by using a mass–spring–damping model. The exact solutions of several modes of a dynamic force microscopy subjected to a compensation of dc voltage, a contact potential difference, the van der Waals force and a tip–sample viscous force are obtained. Some simple and general relations among the Q-factor, the damping ratio, the frequency shift, the tip–sample interacting force, the phase angle, and energy dissipation are discovered. Moreover, the effects of several parameters on the topography and energy dissipation measurement errors are investigated. It is found that

a. Increasing the first frequency shift greatly decreases the topography measurement error due to an unsuitable compensation of dc voltage.

b. If the frequency ratio $s_1 \approx 1$, the topography measurement error will greatly result in the energy dissipation measurement error. But if $\int_{0}^{2\pi} \cos \chi \sqrt{\int_{0}^{s_{1}} - 1}$, the influence of the topography measurement error on the measured phase angle can be neglected.

c. If the frequency shift is increased, although the compensated dc voltage and the tip–sample distance are not applied correctly, an energy dissipation can be accurately calculated by using the measured phase angle.

d. It is better to use the phase angle of the second mode to calculate the energy dissipation than to use the phase angle of the first mode. Although the compensated dc voltage and the tip–sample distance are not correctly applied, the accurate energy dissipation can be determined by measuring the phase angle of the second mode.

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References


