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Nonlocality Effect in Atomic Force Microscopy Measurement and Its Reduction by an Approaching Method

In AFM measurements of surface morphology, the locality is a traditional assumption, i.e., the load recorded by AFM is simply the function of the distance between the tip of AFM and the point on a sample right opposite the tip [Giessibl, F. J., 2003, "Advances in Atomic Force Microscopy," Rev. Mod. Phys., 75, pp. 949–983]. This paper presents that nonlocality effect may play an important role in atomic force microscopic (AFM) measurement. The nonlocality of AFM measurement results from two different finite scales: the finite scale of the characteristic intermolecular interaction distance and the geometric size of AFM tip. With a coupled molecular-continuum method, we analyzed this nonlocality effect in detail. It is found that the nonlocality effect can be formulated by a few dimensionless parameters characterizing the ratio of the following scales: the characteristic intermolecular interaction distance between the AFM tip and the sample, the characteristic size of the tip and the characteristic nano-structure and/or the nanoscale roughness on the surface of a sample. The present work also suggests a data processing algorithm—the approaching method, which can reduce the nonlocality effect in AFM measurement of surface morphology effectively. [DOI: 10.1115/1.1925290]

1 Introduction

The rapid development of the micro/nanoelectromechanical systems (MEMS/NEMS) and some related technologies has led the science of mechanics to focus increasingly on the nanoscale. This is a new challenge and opportunity in the 21st century. Obviously, proper nanometer scale mechanical measurement is one of the prerequisites to the further and solid development of MEMS/NEMS.

In 1986, Binnig and Rohrer were rewarded with the Nobel Prize in Physics for their eximious invention of STM, which provided a breakthrough in our ability to investigate matter on atomic scale. In the same year, Binnig et al. [1] invented the Atomic Force Microscopy (AFM). Nowadays, AFM has become one of the basic instruments commonly used for surface morphology measurements on the nanometer scale. In fact, a number of experiments have been done so far on a variety of layered materials such as graphite [2,3] and boron nitride (BN) [3], ionic crystals such as NaCl [4], and even biological substrates like DNA fragments [5].

It is well known, in AFM measurement, there are various atomic and molecular forces between the tip of instrument and the sample, e.g., van der Waals forces. The force acting on the tip is detected by a microcantilever according to its deformation. At the same time, the instrument adjusts the position of the sample and

the fixed end of the cantilever to keep the force unchanged [6]. The adjustment is taken to interpret the surface morphology of the sample. Actually, this interpretation must be closely related to the assumption of locality in the measurement. The locality assumption means that the load acting on the tip exactly results from the point, on the sample, right opposite the tip apex, regardless of the vicinity of the point. However, in the nanometer scale measurements, the AFM tip is of nanometer magnitude, and in most cases, asperities on a sample surface are of the same order as the tip radius. When we use AFM to detect the surface morphology of a sample, the interaction between the tip and the sample is not only related to the local area of their opposite position, but also related to the status nearby. This may lead to some un-negligible deviation. Then, the locality assumption needs careful re-examining. That is to say, one should ask whether the output given by an AFM is the real surface morphology of a sample.

Many theoretical studies and simulations have been performed for AFM surface morphology measurements. Based on *ab initio* force calculations, Ciraci et al. [7] presented a theoretical analysis of tip-sample interactions in AFM with atomic resolution. Paik et al. [8] obtained the AFM images scanned by many metallic single-atomic tips with molecular dynamics simulation and the Fourier analysis technique. They investigated the elastic surface deformation effects for the W(111) tip and some other bcc metallic tips (Ni and Pt). Abraham et al. [9] investigated the effect of tip structure by using several kinds of multiple-atom tips. They conclude that if the force between the tip and the surface is too repulsive, the resulting image may not be that of the real surface because the surface atoms will significantly relax to lower forces. All of these studies, as well as the works by some other researchers [10–12],

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Fig. 1 Schematic diagram of an AFM tip interacting with a specified rough surface

were carried out on the sample surface that was atomically smooth and the images were obtained under the locality assumption.

However, usually there are some nanoscale structures, such as artificially designed structures in nanodevices as well as the ineluctable disordered roughness on the surface of samples. It is well known that finite tip has limitation to detect the morphology with deep valley [6]. However, it is rarely known that owing to the nonlocality effect even an individual atom tip cannot give exact morphology by means of the assumption of locality. More interestingly, after knowing the nonlocality effect, it becomes possible to obtain the best approximation of the real morphology. In this study, we intend to reveal when the nonlocality effect becomes significant in AFM measurements. By utilizing a coupled molecular-continuum method, which avoids the formidable difficulty in computing ability and time scales in molecular dynamics (MD) simulation [13], we found that nonlocality is induced by the very characteristic intermolecular interaction. Finally, we proposed an algorithm of data processing to reduce the nonlocality effect.

2 Model

We start with the investigation of the nonlocality, by assuming the AFM tip to be a small sphere to approach a specified rough surface, as shown in Fig. 1.

The sample surface is composed of an ideal plane surface with cosine like asperities periodically collocated with amplitude a and wavelength λ . The sample is hemi-infinite in z direction and infinite in x and y direction, and then the sample surface function is

$$z_s = a \cos\left(\frac{2\pi}{\lambda}x\right), \quad (1)$$

as shown in Fig. 1. For simplicity and convenience, the tip is replaced by a sphere with radius R . The separation between the tip and surface is denoted by H , and x_p is the tip position in the horizontal direction.

In our calculation, we consider the intermolecular potential function between the tip and sample as the well-known L-J 6-12 pair potential

$$e(r) = \frac{C r_0^6}{r^{12}} - \frac{C}{r^6}, \quad (2)$$

where the first term of the right-hand side is related to the repulsive potential and the second term attractive potential. C is the constant representing the interaction potential and the parameter r_0 can be considered as a characteristic length in intermolecular interaction, typically taken as 0.3 nm.

The interaction potential energy between the tip and sample W_{ts}^{tot} is composed of 4 parts

$$W_{ts}^{\text{tot}} = W_{tf}^{\text{rep}} - W_{tf}^{\text{att}} + W_{ta}^{\text{rep}} - W_{ta}^{\text{att}}, \quad (3)$$

where the subscripts t , f , and a represent the tip, the hemi-infinite body, and the asperities, respectively, and the superscripts rep and att represent the repulsive and attractive potential energy, respec-

Fig. 2 Schematic of the interaction between the tip and a single particle

tively. From Eq. (3), the z component of the interaction force between the tip and the sample can be expressed by

$$f_{ts}^z = -\frac{\partial W_{ts}^{\text{tot}}}{\partial H}. \quad (4)$$

As we are basically interested in the z component in this study, the z component is denoted by f_{ts} in the following parts of this paper.

3 Coupled Molecular-Continuum Method

To completely calculate (3) and (4), first we must calculate the interaction between the tip and a single particle, as shown in Fig. 2. In Fig. 2, we set up spherical polar coordinates (r, θ, ϕ) at the tip center; R is the tip radius, and S is a microelement in the sphere with coordinates (r, θ, ϕ) . d is the distance between the particle and the tip surface, and l is the distance between the particle and the element, $l^2 = r^2 + (d+R)^2 + 2(d+R)r \sin \theta \sin \phi$. With the assumption of additivity, the net interaction energy of a single particle and the sphere $W_{\text{psph}}^{\text{tot}}$ will be the sum of its interactions with all the molecules in the sphere [14]. Therefore

$$W_{\text{psph}}^{\text{tot}} = C \rho_1 \int_0^R \left(\frac{r_0^6}{l^{12}} - \frac{1}{l^6} \right) r^2 dr \int_0^\pi \sin \theta d\theta \int_0^{2\pi} d\phi, \quad (5)$$

where ρ_1 is the number density of molecules in the sphere.

We can now calculate the total interaction energy of the tip and the hemi-infinite plane surface W_{tf}^{tot} . Following Eq. (5), we obtain

$$W_{tf}^{\text{tot}} = W_{tf}^{\text{rep}} - W_{tf}^{\text{att}} = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \int_{-\infty}^{-a} W_{\text{psph}}^{\text{tot}} \cdot \rho_2 dz, \quad (6)$$

where ρ_2 is the number density of molecules in the sample. For the hemi-infinite plane surface, we can obtain the analytical expression of W_{tf}^{tot} . Similarly we can calculate the interaction energy of the tip and the asperities

$$W_{ta}^{\text{tot}} = W_{ta}^{\text{rep}} - W_{ta}^{\text{att}} = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \int_a^{z_s} W_{\text{psph}}^{\text{tot}} \cdot \rho_2 dz, \quad (7)$$

where z_s denotes the surface of asperities. Substituting Eqs. (5)–(7) into Eqs. (3) and (4), we can obtain the expressions of W_{ts}^{tot} and f_{ts} .

The method of calculation is briefly explained as follows. The force between the tip and the sample is calculated by using the fifth order Gaussian integral method [15], which is one of the most efficient methods of multidimensional numerical integral. Figure 3 shows the process of carrying out the integral through gradually adding up the Gaussian integrals in some more and more subregions. As shown in Fig. 3, we take the point nearest to the tip as the center of the integrating region. First, we calculate the integral in region 1. Then in turn we calculate the integral summations of next circle regions from 2 to 9, 10 to 25, and so on.

Fig. 3 Schematic of the Gaussian integral process

These summations are gradually added up as the final integral and the integral process is terminated if the summation of some circle regions is less than the order of 1.0×10^{-4} , thus we can obtain the f_{ts} for the respective values of H and x_p , i.e., the specified tip position. Since the sample we are concerned with is outspread in the y direction, f_{ts} is independent of y .

We performed the force calculations as mentioned before by choosing a z interval, in which the root of the equation

$$f_{ts} = f_{\text{fixed}} \quad (8)$$

lies for a fixed x_p , where f_{fixed} is the prefixed scanning force. Through the golden search method [15], we can “solve” Eq. (8) within relative error 1% to f_{fixed} . When this procedure is repeated for several x_p values in one period, that is to say, $0 \leq x_p \leq \lambda$, the AFM image with a constant scanning force of f_{fixed} can be obtained. On the other hand, when H is fixed, the constant height image is obtained.

4 Nonlocality Effect in AFM Surface Morphology Measurements

The nonlocality effect in AFM surface morphology measurements means that a finite volume of the sample near to the position right opposite to the tip may contribute to the interaction force between the sample and the tip. This induces that the measured results are the weighted average of these regions instead of the exactly local surface information of the measured point. The reason for this nonlocality effect can be illustrated by the following example (Fig. 4). When the tip apex approaches the sample surface, the main contribution to the tip-sample force comes from the vicinity of point A (see Fig. 4) nearest to the tip, rather than the vicinity of the measured point B. Therefore, even though the distance between the tip and the measure points remains fixed, the force acting on the tip may vary depending on the shape of the surface surrounding the measured points. This can inversely violate the assumption of locality in AFM measurement, i.e., the load recorded by AFM is simply the function of the distance between the tip of AFM and the point right opposite the tip, like point B in Fig. 4 [16].

4.1 Single-Atom Tip. The model of a single-atom tip, which represents the virtual sharpest tip, is calculated for the comparison with the results of more realistic tip models. Specifically we investigate this single-atom tip model in a number of cases with both amplitude a and the wavelength λ of asperities varying from $10r_0$ to $300r_0$. By assuming the tip be diamond and the sample be silicon, we can take the Hamaker constant $A \equiv \pi^2 C \rho_1 \rho_2 = 1.13 \times 10^{-19}$ J in our calculation, provided $A = 1.13 \times 10^{-19}$ J (corresponding to $C = 1.27 \times 10^{-77}$ J m⁶) [17,18]. All the following quantities with length dimension are divided by r_0 , and those with force dimension are divided by C/r_0^7 .

When keeping the vertical separation between the particle and the sample surface fixed to $H \equiv a + 0.78$ and moving the single-atom particle along the surface in one period of asperities, we can

Fig. 4 Schematic of a finite size tip probing a curved sample surface

get the variation curve of the force acting on the particle f_{ps} vs the relative horizontal position x/λ , as illustrated in Fig. 5. From Fig. 5, we can see that, due to the existence of the asperities on sample surface, the force variation is quite sensitive to x/λ especially when the particle is near to the apex of asperities ($x/\lambda \leq 0.2$ or $x/\lambda \geq 0.8$). However, when the particle is a little far from the asperities ($0.2 < x/\lambda < 0.8$), the force acting on the particle becomes very small. This means that even for a single atom tip each asperity has a FINITE influence zone, and the size of the influence zone is decided by the amplitude and wavelength of the asperities and the characteristic interaction distance of L-J pair potential (r_0). In the concerned case ($H \equiv a + 0.78$), for $a = 50$ and $\lambda = 100$ in Fig. 5, the influence zone of each asperity is about 40% λ . Once the particle lies in the influence zone, the force acting on the tip must be nonlocally affected by the asperities, even though the tip is just a single atom!

On the other hand, according to the essential AFM working principle, when fixing the scanning force f_{fixed} in Eq. (8), for every tip position x_p , we can deduce the corresponding separation $H(x_p)$ which represents the “measured” surface morphology of the

Fig. 5 Constant height curve as a single-atom particle moves along the surface in one asperity period (see the inset) with $a = 50$ and $\lambda = 100$

Fig. 6 Comparison of the real (real line) and measured (dash-dotted line) surface morphology scanned by a single particle in one asperity period with $a=50$, $\lambda=100$, and $f_{\text{fixed}}=1.953$

sample. Now let the particle be so close to the sample surface that the AFM can work in contact mode. With the assumption of $f_{\text{fixed}}=1.953$ (0.1 nN), we can obtain the “measured” morphology scanned by the single-atom tip, as shown in Fig. 6. For comparing, we also draw the real surface morphology of the sample in Fig. 6.

From Fig. 6, we can see that in the case of the single-atom tip, the measured and real surface morphology are almost identical, except the slight difference (see the two insets in Fig. 6). In order to characterize the discrepancies between the measured and real surface morphology, we define a distortion parameter

$$S_d \equiv \sqrt{\sum_{i=1}^{N_p} (z_m - z_r)^2} / \sqrt{\sum_{i=1}^{N_p} z_r^2}, \quad (9)$$

where N_p is the number of calculating points in one asperity period, z_m and z_r are the measured and real surface positions, respectively. For $a=50$, $\lambda=100$, and $f_{\text{fixed}}=1.953$ in Fig. 6, $S_d=1.592\%$. This suggests that the nonlocality effect in AFM measurement with a single-atom tip is not very strong when $a \gg 1$ and $\lambda \gg 1$, and the measured results are believable.

However, for deep (with increasing a) and closer (decreasing λ) especially close to characteristic length scale r_0) asperities, the parameter S_d , namely the indicator of the nonlocality effect of the measured results, will increase sharply. Figures 7(a) and 7(b) show the curves of S_d varying with wavelength λ and amplitude a , respectively. These figures indicate that S_d increases with increasing a or decreasing λ , that is to say, the more rough the sample surface is, the more pronounced the nonlocality effect of measured morphology is.

From Figs. 7(a) and 7(b), we can approximately draw out the influence zone in the a - λ space, as illustrated in Fig. 8. Now, it can be concluded that the nonlocality effect of the measured morphology may be significant when the a - λ parameter lies in zone I, while inconspicuous in zone II (at least $\lambda > 10$). From this model of a single-atom tip, where there is a characteristic intermolecular interaction distance r_0 , we can conclude that the nonlocality effect on morphology measurement made by AFM under constant load mode is intrinsic, regardless of the finite size of AFM tip.

Fig. 7 (a) S_d vs λ curves for various a changing from 10 to 40; (b) S_d vs a curves with λ varying from 60 to 100. Both figures are calculated under constant scanning force 0.1 nN.

Fig. 8 Constant $S_d=5.5\%$ curve fitted by the polynomial. The points are calculated under constant scanning force 0.1 nN.

4.2 Finite Size Tip. In this section, we give the results of calculations on the nonlocality effect resulting from the finite size tip. Suppose the sphere tip has finite size $R=10$ but the other parameters remain the same as those in Sect. 4.1. Following the same way we did in the cases of a single-atom tip, we can calculate the “measured” surface morphology using the finite size tip, as shown in Fig. 9.

Figure 9 clearly indicates that there are significant discrepancies between the measured and the real surface morphology using the finite size tip. For the tip of $R=10$, $a=50$, and $\lambda=100$ in Fig. 9, S_d increases up to 22.62% while for a single-atom tip S_d is 1.592% only. Notice that in this case the sphere tip is $2R/a \sim 2.5$ and $2R/\lambda \sim 0.2$ only, but the variation of $S_d=22.62\%$ has been quite considerable. This S_d increase occurs for all other parameters of a and λ . Comparing to the measured results by the single-atom tip, we realize that the considerable difference between the calculated results and the real surface morphology is mainly induced by the geometrical structure of the sample surface plus the finite size of the tip. Therefore, when using a realistic tip with finite size to scan the surface, we must consider the nonlocality effect induced by the AFM tip on the measurement surface morphology.

Fig. 9 Comparison of the real (real line) and measured (dashed-dotted line) surface morphology scanned by a finite size tip with $R=10$ in one asperity period with $a=50$ and $\lambda=100$ under constant load $f_{\text{fixed}}=1.953(0.1 \text{ nN})$

Fig. 10 Comparison of the approaching and the scanning results of surface morphology. The former are calculated by the approaching method and the latter are scanned by the single-atom tip under constant force 0.1 nN. Both a and λ are 10.

5 Approaching Method to Improve Measurement

As shown in Fig. 8, even in the case of single-atom tip, for some a and λ values, S_d is greater than 5%. For instance for $a=10$ and $\lambda=10$, $S_d=17.14\%$, as shown in Fig. 7(a). This is intolerable in practical AFM measurements. In this section, we propose an approaching method, different from that made by Tang, Joachim, and Devillers [10], to deal with the “measuremental” data for the sake of reducing the nonlocality-induced relative error between the measured and real surface morphology.

5.1 Single-Atom Tip. First, let us introduce the approaching method with the measurement with a single-atom tip. For a given x_p , the tip-sample force f_{ps} can be obtained for several H values. Then suppose that the $f_{ps}(H)$ function can be fitted from these data by a power law

$$p/(H-q)^\gamma, \quad (10)$$

where p , q , and γ are the three parameters to be fitted. It is well known that the tip-sample force will certainly tend to infinity as the tip is approaching the sample surface. Therefore, as the exponential function $p/(H-q)^\gamma$ has a singularity at $H=q$, the fitted parameter q is actually the position of the real surface morphology, which however cannot be realized in practical AFM measurements. Then, the fitting function $f(x_p)$ gives a measurement of surface morphology approaching the real one. Figure 10 shows the results of surface morphology using this approaching method for every x_p in one asperity period with 40 data of H .

In Fig. 10, by using the proposed approaching method, S_d decreases from 17.14% (corresponding to the scanned results with a finite size tip) to 4.56%. The reduced error is acceptable and this approaching method is efficient in reducing the nonlocality effect involved in the measured results. Figure 10 clearly indicates that the method provides a powerful technique to reduce the nonlocality effect and then to obtain higher fidelity surface morphology from a series of measuremental data in AFM measurements.

5.2 Finite Size Tip. Similarly as we performed in Fig. 10, we can obtain the first approaching results of surface morphology scanned by finite size tip, as shown in Fig. 11. Figure 11 shows that, although the first approaching result reduces S_d from 78.14% to 49.12%, it is not yet closely approaching the real surface morphology. The reason can be explained by Fig. 12.

When a tip with radius R is probing the site B on the surface in the vertical (z) direction, the real contact position between the tip

Fig. 11 Comparison of the approaching and the scanning results of surface morphology. The former two are calculated by the first and second approaching methods respectively and the latter are directly scanned by the finite size tip with $R=1$ under constant force 0.1 nN. Both a and λ are 10.

and the surface is point A rather than point B. This induces that the vertical force between them tends to infinity before the tip touches the site B. Actually, for each location x_p , there exists a $H_{\min}=q$ corresponding to the lowest position the tip can reach in the first approaching. Thus the curve of $H_{\min}$ versus x_p is called the first approaching surface morphology. Accordingly, the relative error between this $H_{\min} \sim x_p$ curve and the real surface morphology is the minimum we can reach in the first approaching when using a finite size tip to scan the surface. Our approaching results in Fig. 11 are nearly the same as the $H_{\min} \sim x_p$ curve. Figure 11 also indicates that the geometrical structure of the tip can bring profound nonlocality effect on the measured results and that this effect is ineluctable. This has important implications for practical AFM surface morphology measurements.

As noted in Fig. 11 S_d is still as high as nearly 50%, which is unacceptable. However, since the finite size R of the tip is known, we can go further to improve the first approaching results in Fig. 11. The secondary approaching method to reduce S_d is illustrated in Fig. 13. Here we take a linear approximation AC of the curved surface AB, where C is taken to interpret the point B on the real surface. Following the simple geometrical relation, we have

$$H_C = q - R/\sin \alpha + R, \quad (11)$$

where q is the fitted parameter to interpret $H_{\min}$ and α is the included angle between AC and O'B and can be determined by

Fig. 12 Schematic of a finite size tip contacting the sample

Fig. 13 Schematic of the secondary approaching method. The tip contacts the surface at point A and B is the point opposite to the tip. AC is the tangent of the sample surface.

previous approaching results. By this means, S_d has a tremendous decrease from 49.12% to 13.73% (see Fig. 11). This indicates that the secondary approaching method we proposed is very efficient in deducing the nonlocality effect owing to finite tip size on the morphology measurements.

Now we briefly summarize the approaching method of data processing as follows. For every measured point (x_p), the method needs several measuremental data to fit the power function of $f_{ts} = p/(H-q)^\gamma$. From the fitting, we can obtain q values $q(x_p)$, which represent the first approaching surface morphology. For the single-atom tip, that is enough. For the finite size tip, we need to deal with the approaching results once more by expression $H_C = q - R/\sin \alpha + R$ to further reduce the error resulting from the finite size of tip. To perform this secondary approaching, one needs the tip radius and the previous approaching results to calculate the value of α only.

However, it should be noted that in the analysis, both tip and sample are assumed to be undeformed. The effect of contact deformation on the measurement needs some approximate models of contact mechanics [19].

6 Summary

The most crucial point in experimental measurements is that the signals directly recorded are usually the coupled information of both sample and instrument, hence how to extract the exact information of the concerned sample is a prominent problem in nanometer scale measurements. Since locality is taken to be an essential but implicit assumption, the significance of nonlocality is almost disregarded in practice. Actually, as shown in this paper, even for a single atom tip to scan a not very rough surface (with roughness height $a=50$ and wavelength $\lambda=100$, normalized by atom spacing), the distortion parameter S_d still can be 1.592% resulting from the nonlocality effect. Therefore, it is really important to bear in mind that the nonlocality is an intrinsic effect in nanometer scale measurements.

By using a coupled molecule-continuum method, we found that the following effects of nonlocality need special attention in data processing of AFM morphology measurements, especially for highly curved surfaces:

- (1) The nonlocality of AFM measurements basically results from the intrinsic characteristic length scale of intermolecular interaction. This is the reason why the morphology of sample surface even measured by a single atom probe can still be affected by the nonlocality effect.
- (2) The finite geometric size of AFM tip, coupled with the above intrinsic length scale of intermolecular interaction

makes the nonlocality effect even more severe and complicated in practical AFM morphology measurements. For instance, for a finite tip ($R=10$) to scan the same sample as that measured by single atom tip, the distortion parameter can go up to 22.62% due to the nonlocality effect.

- (3) In addition, the nonlocality effect can be extremely exaggerated by high and dense asperities of sample surface. For instance, for a rough surface ($a=10$ and $\lambda=10$), the distortion parameter S_d can go up to 17.14% by a single atom tip and to 78.14% for the finite tip ($R=10$). This effect can even make exact measurement of surface morphology quite impossible.
- (4) In order to perform an effective data processing to gain high fidelity of surface morphology, by taking nonlocality into account we proposed an approaching method, which can significantly reduce the nonlocality effect on morphology measurement, especially for finite size tip. For instance, for the rough surface ($a=10$ and $\lambda=10$), the distortion parameter S_d can decrease from 17.14% to 4.56% for single atom tip and from 78.14% down to 13.73% for a finite tip ($R=10$).

In one word, it is crucially important to notice that the nonlocality effect is intrinsic as well as significant in nanometer scale measurements, such as AFM surface morphology measurements.

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