Sample trapped charge induced signals in tapping-mode atomic force microscopy

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Abstract. AFM (Atomic force microscope) has been used to measure the surface topography and electrochemical properties of the sample by the interaction between the tip on the cantilever and the sample. However, when there is a charge in the sample, an induced charge will be generated inside the tip, which will generate a new attractive force between the tip and the sample and reduce the amplitude of the tip. We found that the average amplitude of the tip decreased by about 1 nm in tapping mode AFM. As the amplitude decreasing, AFM keeps the amplitude constant by adjusting $z_0$ with negative feedback in tapping mode. So, the average charge density will affect the measurement of surface topography.

1. Introduction
AFM is a new type of instrument with high resolution at atomic level invented after scanning tunneling microscope. It can detect the physical properties of various materials and samples in the atmosphere and liquid environment, including morphology, or directly manipulate them. AFM has been widely used in semiconductor, nano-functional materials, biology, chemical industry and food, pharmaceutical research and research institutes of various nanoscale related disciplines, and has become a basic tool for nano-science research [1,2,3].

TM-AFM (Tapping-mode atomic force microscopy) is a dynamic imaging mode in which the tip is oscillated close to its resonance frequency and interacts with the sample once in every oscillation. In this mode of imaging, the cantilever oscillation amplitude is kept constant by the feedback loop and the feedback signal to the piezoelement is recorded as a topography image.

The purpose of this experiment is that when AFM is used to measure the surface topography of the sample, if there are charges on the surface of the sample, the induced charge will be generated inside the tip, and the attractive force will be generated between the charges on the surface of the sample and the induced charge. If the attractive force is ignored, AFM will raise the tip in order to keep the amplitude constant. This will change the measured surface topography. In this simulation experiment, the tip is assumed to be a metal ball, and the charges on the sample surface are distributed in a certain way. In the case of maintaining a relatively stable TM, we find that, as the gradual increase of charge density, the amplitude of the tip will gradually decrease, and the maximum decrease amplitude can be about 1 nm.
2. Forces analysis in AFM

2.1 DMT contact mode

In this work, we use DMT (Dejarguin-Muller-Toporov) contact model to model the interaction of tip and sample [4,5]. Regardless of the charge on the sample surface, the tip will be subjected to two kinds of forces in TM-AFM. When the tip is far away from the sample surface, it will be subjected to van der Waals force (attraction force).

As the tip close to the sample, repulsive forces emerge in addition to attractive forces. And the repulsive force is called Hertz [6], by combining these two effects.

The coupled differential equations of motion for the system described above can be written as

\[ m \ddot{Z} + \gamma \dot{Z} + kZ = F_{ts} \sin(\omega t) \]  

In these equations, \( F_{ts} \) is the amplitude of cantilever driving force, \( Q_c \) is the cantilever quality factor and \( \omega_{o_c} \) is the fundamental flexural resonance frequency of the cantilever. In addition, \( F_{ts} \) denotes the tip-sample interaction force and is given by

\[ F_{ts} = -\frac{HR}{6(Z_0 + Z_c)^2} \quad Z_0 + Z_c \geq a_0 \]  

\[ F_{ts} = -\frac{HR}{6a_0^2} + \frac{4}{3}E'\sqrt{R}(a_0 - Z_0 - Z_c)^3 \quad Z_0 + Z_c < a_0 \]

The motion amplitude of the tip equation (1) can be calculated by explicit Runge-Kutta methods [7].

2.2 Electrostatic Forces analysis in AFM

When there are charges in the sample, the tip is close to the surface of the sample, and the induced charge will be generated inside the tip. It is assumed that the tip is a metal ball, and the area of charge distribution affected by the sample surface below the tip is a circle with a radius of 3R [8]. When the radius is greater than 3R, the increased charge is far away from the tip, and the tip produces very weak attractive force, which has negligible effect on the amplitude.

First, it is assumed that \( n \) charges (electrons) are shared equally on the diameter of a 3R-radius circle. Each charge \( q \) in the sample can produce the corresponding induced charge \( q' \). Then calculate the downward attractive forces of each charge to the tip, and sum them.

![Figure 1. Influence of surface charge distribution on tip](image)

Figure 1. Influence of surface charge distribution on tip
\[ \theta = \arctan \left( \frac{k N \cdot 3R}{R + z} \right) \]  

(4)

\[ a = \frac{R^2}{(R + z)/\cos \theta} \]  

(5)

\[ F_{et} = - \sum_{i=1}^{N} \frac{kq^2 R}{(R + z)/\cos \theta} \cdot \cos \theta \cdot \left( \frac{R + z}{\cos \theta - a} \right)^2 \]  

(6)

Then, expanding it to N times, AFM obtains the change of tip amplitude.

\[ F_{et} = -n \cdot \sum_{i=1}^{N} \frac{kq^2 R}{(R + z)/\cos \theta} \cdot \cos \theta \cdot \left( \frac{R + z}{\cos \theta - a} \right)^2 \]  

(7)

According to this distribution, the charge distribution is not uniform on the sample with 3R radius under the tip. The closer to the lower part of the tip, the sample has the higher charge density. Therefore, this kind of charge distribution can increase the attraction of the surface charge of the sample to the tip, and the amplitude will be decreased [9]. If the charge distribution is uniform, it is not difficult to find out that the tip will be much less attractive.

Irrespective of the charges in the sample’s surface, the tip is only attracted by van der Waals force. The magnitude of the force is on the order of -10 to -12. When considering the surface charge of the sample, the magnitude of the force is on the order of -8 to -9 [10]. When the tip closes to the sample surface, the attractive force increases about 100 times in figure 2.

When increasing the value of \( n \), the amplitude of the tip will decrease, so we can get the relationship between the average charge density of the sample surface below the tip and the amplitude of the tip.
Table 1. The relationship between average charge density and amplitude of the tip

| n   | 0     | 500   | 600   | 1000  | 1100  | 1200  |
|-----|-------|-------|-------|-------|-------|-------|
|     |       |       |       |       |       |       |
| average charge density (e/ cm²) | 0     | 0.707 × 10¹⁴ | 0.849 × 10¹⁴ | 0.990 × 10¹⁴ | 1.556 × 10¹⁴ | 1.698 × 10¹⁴ |
| amplitude of the tip (nm)      | 35.10 | 34.26 | 34.24 | 34.09 | 34.04 | 33.85 |

We found that when \( n = 1200 \), the tip amplitude will be reduced by 1.25 nm. The average charge density of the sample is \( 1.698 \times 10^{14} \text{e/cm}^2 \).

As the amplitude decreasing, AFM keeps the amplitude constant by adjusting \( z_0 \) with negative feedback in tapping mode. When AFM measures the surface morphology of the sample, the charges on the surface of the sample will lead to the AFM false feedback and lead to the tip elevation, which makes surface topography inaccurate. Through simulation, we find out the relationship between the average charges density of sample and the change of \( z_0(\Delta z_0) \).

![Figure 3. The relationship between the average charges density of sample and the \( \Delta z_0 \)](image)

It can be seen from the figure 3. that with the increasing of the average charge density of the sample, \( z_0 \) is increasing. When the average charge density equals \( 1.556 \times 10^{14} \text{e/cm}^2 \), \( \Delta z_0 \) is 1.2 nm. In addition, a list of parameter values used in calculations is given in [10].

3. Conclusion

The simulation experiment is realized by MATLAB, we draw the following conclusions: (1) When there are charges on the surface of the sample, the tip will be gravitated and the amplitude of the tip will be reduced; (2) The larger the charge density near the tip is, the greater the attractive force will be generated and the smaller the tip amplitude will be. In TM-AFM, the maximum amplitude will be reduced by about 1 nm; (3) In tapping mode, when the average charge density equals \( 1.556 \times 10^{14} \text{e/cm}^2 \), the tip will raise 1.2 nm by negative feedback in tapping mode, which causes surface topography inaccurate.

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