Proceedings of the 2nd IEEE International
Conference on Nano/Micro Engineered and Molecular Systems
January 16 - 19, 2007, Bangkok, Thailand

A Study on Theoretical Nano Forces in AFM Based Nanomanipulation

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Abstract **As it is important to understand the basic mechanics principle in nanofabrication process, much research has been done about nano mechanics with different tools in different nano enviroments, and various kinds of nano force formula have been proposed. However, as the special case of AFM based nanomanipulation is considered, little about its mechanics principle under the micro probe's operation is known, such as what kinds of nano forces are the decisive factors and how they work, which are important to perform accurate control in nanomanipulation. To explore this subject, nano forces among tip, substrate and particle are analyzed, and simulation & experiments are performed to verify the rationality of the analysis.**

Keywords- Nano force analysis, force curve, nanomanipulation, atomic force microscope (AFM)

I. INTRODUCTION

With the development of nano fabrication technology, it becomes important to understand the basic mechanics and physics principle in nanofabrication process. For that, much research work has been done on nano mechanics in different nano environments, and various kinds of nano force formula have been proposed [1~5]. However, it is very difficult to make sure what kinds of nano forces play important role and how they work in different conditions. And here as the special case of AFM based nanomanipulation is considered, so little about its mechanics principle under the micro probe's operation is known to us all, such as what kinds of nano forces are the decisive factors and how they work, which are important to perform accurate control in nanomanipulation.

To explore this subject, nano forces among tip, particle and substrate in nanomanipulation are analyzed, and simulation & experiments will be performed to verify the rationality of the analysis.

II. CONFIGURATION OF MAIN NANO FORCES

Although there exist various nano forces in different nano conditions, in the case of AFM based nanomanipulation with a micro probe, what are the main forces and how they work remain not very clear. Here based on the researchers' research result [1~5] and our own nanomanipulation experience, and with the consideration of basic nano forces and other effect factors such as wet environment and electrostatic charge, the crucial nano forces can be summarized as Van der Waals force, repulsive contact force and nano frictional force which are three basic nano forces, and capillary force aroused by wet environment, and electrostatic force caused by the electrostatic charge. All these nano forces can be cataloged into attractive, repulsive and frictional force according to their effect in nanomanipulation. To prevent probe from sliding above the particle during manipulation, the probe will be pushed on the substrate to perform manipulation after it was located nearby the particle, thus the probe will contact with particle and substrate, and the nano forces among tip, substrate and particle can be described as shown in Fig.1.

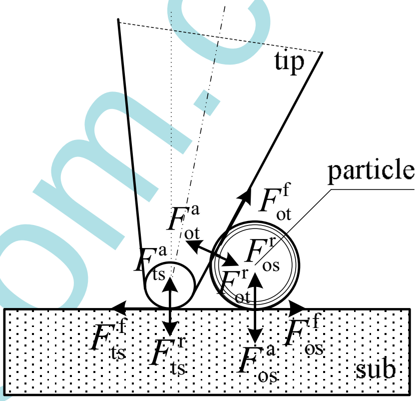

Fig.1 Interactive forces among tip, particle and substrate

where F^f_{ts}、F^f_{os}、F^f_{to} are the nano frictional force, F^a_{to}、F^a_{os}、F^a_{ts} are attractive force which consists of attractive Van der Waals force, capillary force and attractive electrostatic force, and F^r_{ts}、F^r_{ot}、F^r_{os} are repulsive force composed of repulsive contact force, repulsive Van der Waals force and repulsive electrostatic force. And the tip is viewed as a ball with radius about 10nm, and the particles are commonly ball-like or tube-like particles such as gold particle, carbon nanotube and etc.

With the consideration of these five kinds of nano forces, the detailed analysis will be put forward in the following.

III. WORKING PRINCIPLE OF NANO FORCES

A. Van der Waals Force

Van der Waals force originates form electromagnetic forces between two dipoles, and it depends on the two particles' distance, material characteristics parameters and geometry shapes, and whether it is adhesive or repulsive force depends mainly on the distance and also the material's Hamaker constant [6]. For common manipulation particles, such as ball-like or tube-like particles (carbon nanotube), Van der Waals force will be analyzed in detail in this section [1,4].

This project was funded by the Chinese NSF (Project code: 60575060, 60575050 and 60635040)

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1) Between particle and tip

As the contact area on tip is relative large compared with nanometer scale as shown in Fig.1, it can be viewed as a flat plane, and Van der Waals force between the ball-like particle and the tip can be represented as

$$F_{\mathrm{to}}^{\mathrm{v}} = \frac{A_H\, r_{\mathrm{o}}}{6\, h_{\mathrm{to}}{}^2} \tag{1}$$

Likewise, Van der Waals force between the tube-like particle and the tip can be presented as

$$F_{\mathrm{to}}^{\mathrm{v}} = \frac{A_H \sqrt{r_{\mathrm{o}}}}{8\sqrt{2} h_{\mathrm{to}}{}^{5/2}} \tag{2}$$

2) Between particle and substrate

Van der Waals force between the ball-like particle and the substrate can be

$$F_{\mathrm{os}}^{\mathrm{v}} = \frac{A_H r_{\mathrm{o}}}{6 h_{\mathrm{os}}{}^2} \tag{3}$$

While Van der Waals between the tube-like particle and the substrate can be

$$F_{\mathrm{os}}^{\mathrm{v}} = \frac{A_H \sqrt{r_{\mathrm{o}}}}{8\sqrt{2} h_{\mathrm{os}}{}^{5/2}} \tag{4}$$

3) Between tip and substrate

Van der Waals force can be presented as

$$F_{\mathrm{ts}}^{\mathrm{v}} = \frac{A_H r_{\mathrm{t}}}{6 h_{\mathrm{ts}}{}^2} \tag{5}$$

where in the formula (1)~(5), A_H is Hamaker constant which can be positive or negative [6], r_{t} is tip's radius, r_{o} is particle's radius, h_{to} is the distance between the tip and the particle, h_{ts} is distance between the tip and the substrate, and h_{os} is the distance between the particle and the substrate.

B. Repulsive Force

During nanomanipulation, the tip, the particle and the substrate contact with each other and there will be repulsive contact forces among them, generally this kind of forces is crucial in nanomanipulation and here it will be analyzed in detail [3].

1) Between particle and tip

$$F_{\mathrm{ot}}^{\mathrm{r}} = \sqrt{2k_{\mathrm{ot}}^{\mathrm{s}} q_{\mathrm{ot}} r_{\mathrm{ot}}{}^3 / r_{\mathrm{o}}} + k_{\mathrm{ot}}^{\mathrm{s}} r_{\mathrm{ot}}{}^3 / r_{\mathrm{o}} \tag{6}$$

where $k_{\mathrm{ot}}^{\mathrm{s}} = 4/(3\pi k_{\mathrm{ot}}^{\mathrm{e}})$, and $k_{\mathrm{ot}}^{\mathrm{e}}$ is the effective spring constant between the particle and the tip, and it can be presented as $k_{\mathrm{ot}}^{\mathrm{e}} = k_{\mathrm{o}} + k_{\mathrm{t}}$; $q_{\mathrm{ot}} = 3\pi r_{\mathrm{o}} W_{\mathrm{ot}}{}^{\mathrm{a}}$, where $W_{\mathrm{ot}}^{\mathrm{a}}$ is the adhesive energy density of the interface between particle and tip, and it can be described as $W_{\mathrm{ot}}^{\mathrm{a}} = \dfrac{A_H}{12\pi h_{to}^2}$; r_{ot} is the contact radius between the particle and the tip, and it can be represented as $r_{\mathrm{ot}} = (6\pi r_{\mathrm{o}}{}^2 W_{\mathrm{ot}}^{\mathrm{a}} / k_{\mathrm{ot}}^{\mathrm{e}})^{1/3}$.

2) Between particle and substrate

$$F_{\mathrm{os}}^{\mathrm{r}} = \sqrt{2k_{\mathrm{os}}^{\mathrm{s}} q_{\mathrm{os}} r_{\mathrm{os}}{}^3 / r_{\mathrm{o}}} + k_{\mathrm{os}}^{\mathrm{s}} r_{\mathrm{os}}{}^3 / r_{\mathrm{o}} \tag{7}$$

where $k_{\mathrm{os}}^{\mathrm{s}} = 4/(3\pi k_{\mathrm{os}}^{\mathrm{e}})$, and $k_{\mathrm{os}}^{\mathrm{e}}$ is the effective spring constant between the particle and the substrate, and it can be presented as $k_{\mathrm{os}}^{\mathrm{e}} = k_{\mathrm{o}} + k_{\mathrm{s}}$; $q_{\mathrm{os}} = 3\pi r_{\mathrm{o}} W_{\mathrm{os}}^{\mathrm{a}}$, where $W_{\mathrm{os}}^{\mathrm{a}}$ is the adhesive energy density of the interface between the particle and the substrate, and it can be described as $W_{\mathrm{os}}^{\mathrm{a}} = \dfrac{A_H}{12\pi h_{\mathrm{os}}^2}$; r_{os} is the contact radius between the particle and the substrate, and it can be represented as $r_{\mathrm{os}} = (6\pi r_{\mathrm{o}}{}^2 W_{\mathrm{os}}^{\mathrm{a}} / k_{\mathrm{os}}^{\mathrm{e}})^{1/3}$.

3) Between tip and substrate

$$F_{\mathrm{ts}}^{\mathrm{r}} = \sqrt{2k_{\mathrm{ts}}^{\mathrm{s}} q_{\mathrm{ts}} r_{\mathrm{ts}}{}^3 / r_{\mathrm{t}}} + k_{\mathrm{ts}}^{\mathrm{s}} r_{\mathrm{ts}}{}^3 / r_{\mathrm{t}} \tag{8}$$

where $k_{\mathrm{ts}}^{\mathrm{s}} = 4/(3\pi k_{\mathrm{ts}}^{\mathrm{e}})$, $k_{\mathrm{ts}}^{\mathrm{e}}$ is the effective spring constant between the tip and the substrate, and it can be presented as $k_{\mathrm{ts}}^{\mathrm{e}} = k_{\mathrm{t}} + k_{\mathrm{s}}$; $q_{\mathrm{ts}} = 3\pi r_{\mathrm{t}} W_{\mathrm{ts}}^{\mathrm{a}}$, $W_{\mathrm{ts}}^{\mathrm{a}}$ is the adhesive energy density of the interface between the tip and the substrate, and it can be described as $W_{\mathrm{ts}}^{\mathrm{a}} = \dfrac{A_H}{12\pi h_{\mathrm{ts}}^2}$; r_{ts} is the contact radius between the tip and the substrate, and it can be represented as $r_{\mathrm{ts}} = (6\pi r_{\mathrm{t}}{}^2 W_{\mathrm{ts}}^{\mathrm{a}} / k_{\mathrm{ts}}^{\mathrm{e}})^{1/3}$.

C. Nano Frictional Force

Classical frictional force can be presented as

$$F^f = \mu N \tag{9}$$

where μ is the frictional coefficient, and N is the normal force.

During nanomanipulation, as there exists micro deformation at the contact area, there will be another force component added into the frictional force, and it can be described as [7]

$$F^f = s_{\mathrm{c}} A + \mu N \tag{10}$$

where s_{c} is the critical shear stress, and A is the contact area with radius being

$$r_C = \frac{r}{k}\left[N + 6\pi r\gamma_{\mathrm{SS}} + \sqrt{12\pi r\gamma_{\mathrm{SS}} N + (6\pi r\gamma_{\mathrm{SS}})^2}\right] \tag{11}$$

where $r = r_1 r_2/(r_1 + r_2)$, γ_{SS} is the contact surface energy , and k is the effective spring constant

Thus the total frictional force can be described as

$$F_f = \pi s_c \frac{r}{k}\left[N + 6\pi r\gamma_{SS} + \sqrt{12\pi r\gamma_{SS}N + (6\pi r\gamma_{SS})^2}\right] + \mu N \quad (12)$$

D. Capillary Force

As nanomanipulation experiments are always performed in atmosphere condition, micro liquid membrane will form between particle and substrate as particle deposits on the substrate, the capillary force between particle and substrate shown in Fig.2 can be described as [2][4]

$$F_{os}^{c} = 4\pi r_o(\gamma_{LS}\cos\theta + \gamma_{SS}) \quad (13)$$

where r_o is the radius of the particle, θ is the contact angle, γ_{LS} is surface potential at the liquid-solid interface, and γ_{SS} is surface potential at the solid-solid interface.

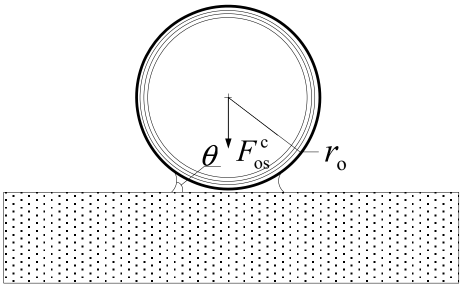

Fig.2 Capillary force applied on particle

For micro liquid membrane seldom forms on the particle's upper surface, there will be no capillary force between the tip and the particle.

E. Eletrostatic Force

As there will be some electrical charge accumulated on the surface of particle or tip, the particle manipulated is prone to adhere on the tip due to electrostatic attractive force and it will fail the manipulation, thus the electrostatic force should be considered and will be analyzed here [8][9].

1) Between particle and tip

When the particle is ball-like, the electrostatic force between the particle and the tip will be

$$F_{to}^{es} = \kappa_{to} r_o Z_{to} e^{\kappa_{to}h_{to}} \quad (14)$$

While to tube-like particle, it can be

$$F_{to}^{es} = \kappa_{to}^{3/2}\sqrt{r_o / 2\pi Z_{to}}\, e^{\kappa_{to}h_{to}} \quad (15)$$

where κ_{to}^{-1} is the Debye length and Z_{to} is the characteristic parameter of the tip and the particle.

2) Between particle and substrate

The electrostatic force between the ball-like particle and the substrate will be

$$F_{os}^{es} = \kappa_{os} r_o Z_{os} e^{\kappa_{os}h_{os}} \quad (16)$$

While to the tube-like particle, the electrostatic force will be

$$F_{os}^{es} = \kappa_{os}^{3/2}\sqrt{\frac{r_o}{2\pi}}Z_{os} e^{\kappa_{os}h_{os}} \quad (17)$$

where κ_{os}^{-1} is the Debye length and Z_{os} is the characteristic parameter of the particle and the substrate.

3) Between tip and substrate

The electrostatic force can be

$$F_{ts}^{es} = \kappa_{ts} r_t Z_{ts} e^{\kappa_{ts}h_{ts}} \quad (18)$$

where κ_{ts}^{-1} is the Debye length and Z_{ts} is the characteristic parameter of the tip and the substrate.

IV SIMULATION AND EXPERIMENT OF FORCE-DISTANCE CURVE

To verify the effectiveness of the analysis proposed above, here simulation and experiment of classic force-distance curve will be performed.

The experiment process of classic force curve will be as follows. With the probe controlled to approach the substrate vertically, the cantilever will deflect downward by the attractive force between the tip and the substrate, and at the contact point the tip will jump onto the substrate. Continually approaching the substrate, the cantilever will deflect upward slowly mainly by the repulsive contact force until the deflection reaches a predefined lever. Then the tip is controlled to leave the sample, and the cantilever will jump upward when the tip leave the substrate abruptly, which means that the spring restoring force of the cantilever overcomes the strong attractive force between the tip and the substrate. And after that the experiment of force curve is finished with the tip continually leaving the substrate. In the experiment, the force acting on the tip is calculated according to the cantilever deflection and its spring constant, and thus to obtain the dependent curve of the normal force on the distance between the tip and the substrate, which is abbreviated as force curve, and the classic force curve is shown in Fig. 3 [10].

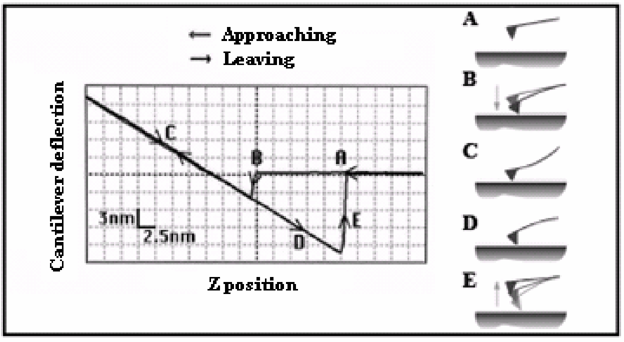

Fig.3 Classical force curve

As the real parameters in the complex nanoenvironment are difficult to get, here simulation and experiment will be performed on a relative simple experiment condition.

Firstly, the simulation is performed according to the actual experiment condition described as follows, Si probe and Si substrate are grounded to release the electrostatic charge for minimizing electrostatic force, the experiment condition keeps dry to minimize the capillary force and the lateral frictional force can be ignored as the probe moves vertically, thus the crucial forces between the tip and the substrate are mainly Van der Waals force and repulsive contact force. With the parameters set as the tip radius equal to 10nm, Hamaker constant of Si equal to 6*10^-20J and spring constant of Si equal to 214Gpa, the simulated force curve can be obtained as shown in Fig. 4.

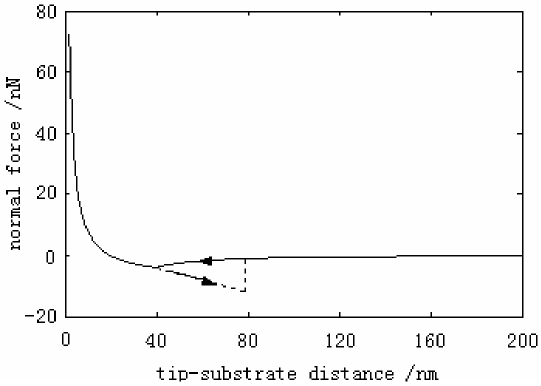

Fig.4 Simulated result of force curve

In Fig.4, the real line represents the process of the probe approaching the sample, while dotted line represents the process of the probe leaving the sample, and here these two lines are partly super-positioned.

Comparing Fig.4 and Fig.3, we can see that the change trend of the two force curves is similar with each other, which preliminarily verified the rationality of the analysis.

Secondly, according to the experiment condition described above, force curve experiment is performed with program-controlled probe motion by AFM based robotic nanomanipulation system shown in Fig. 5 [11], and the force curve is obtained as shown in Fig. 6.

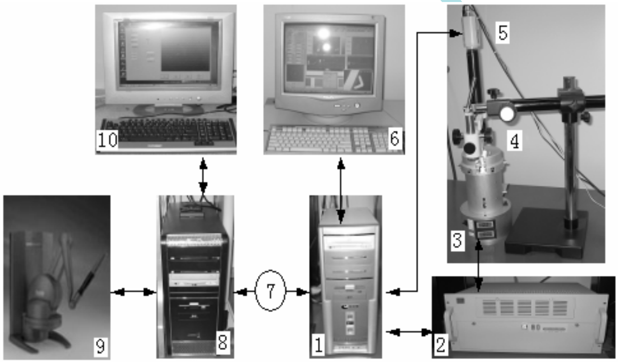

Fig.5 AFM based robotic nanomanipulation system

where in Fig. 5, 1 is the AFM control computer, 2 is the CSPM 2000wet controller, 3 is the AFM head, 4 is the optical microscope, and 5 is the CCD camera, 6 is the monitor for imaging and optical vision, 7 is the Ethernet device, 8 is the control computer of haptic device, 9 is the haptic device, and 10 is the monitor for manipulation interface.

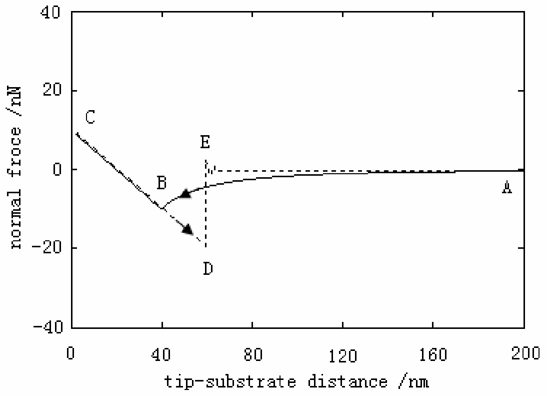

Fig.6 Experimental result of force curve

In Fig. 6, the real line represents the probe approaching, while the dashed line represents the probe leaving the sample. During probe's approaching, the force in line AB mainly consists of Van der Waals force, and with attractive force increasing the deflection also increases until the tip jumps onto the sample, where the capillary force still makes effect as it can not be kept absolutely dry in the experiment. And then the repulsive contact force makes main effect in section BC, which results in the cantilever' upward deflection. While during the probe's leaving, section CD represents that the repulsive force turns into the resultant effect of Van der Waals force and capillary force, until to the point D where the tip jumps off the sample. And finally in section EA the Van der Waals force acts on the tip, which is a little different from section AB where the residual electrostatic force still exists. In addition, what is practically obtained on the vertical axis is the signal of position sensitive detector (PSD) reflecting the cantilever's deflection, while on the lateral axis the actuating voltage, and here the force and displacement are calibrated by gratings [11].

And comparing Fig. 6 and Fig. 4, one can see that the trend and scale of the two curves are consistent with each other, which further verified the rationality of the analysis. However, for some parameters in nano forces, such as some material characteristics parameters, geometrical parameters and etc., can not be accurately obtained, there exits some difference between the theoretical and experimental results, which further demonstrates the necessity of nano forces' actual measurement [11].

V. CONCLUSION

As AFM based nanomanipulation with the micro probe is considered, nano forces among tip, substrate and particle and their working effects are analyzed in detail, and the simulation and experiment are performed to verify the effectiveness of the analysis, which is helpful for understanding nano mechanics principle of the AFM probe's operation and performing accurately nanomanipulation.

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