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An Analysis on Nano-scale Tip-Sample Interaction Forces in Atomic Force Microscopy

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Abstract

Recently, the capability of capturing images with a nanometric resolution has considerably increased the amount of developments in nanotechnologies. One of the most appealing tools to make this capability is known as Atomic Force Microscope (AFM). Thus, dynamic analysis of this kind of instrument is a significant and important task, especially when AFM operates in adjacent of a sample. By the current research, an analysis on tip-sample interaction forces in tapping mode of AFM is presented. Having a correct understanding of the tip-sample interaction forces is very important in obtaining high-precision images and reliable data. Identifying these nanoscale forces makes a crucial role in dynamic analysis of AFM, and makes it able to operate in a wide range of applications such as semi-conductors, materials and manufacturing, polymers, biology and biomaterials. Consequently, this paper presents a review on tip-sample interaction forces in tapping mode atomic force microscopy.

Key Word and Phrases
Atomic Force Microscopy, Tapping Mode, Tip-Sample Interaction Forces, Nano-Contact Mechanics Models, Nanoscale.

1. Introduction

The atomic force microscope system has become a useful tool for measurements of parameters of micro structures and unraveling the intermolecular forces at nanoscale level with atomic-resolution characterization [1], and can be utilized in a wide range of applications such as semi-conductors, materials and manufacturing, polymers, biology and biomaterials [2]-[5]. Typically, AFMs are operated in three open-loop modes: non-contact mode, contact mode, and tapping mode. In the contact mode, the cantilever tip remains in contact with the target sample, and interaction forces are monitored. Alternatively, the non-contact mode is utilized by moving the cantilever slightly away from the sample surface and oscillating the cantilever at or near its natural resonance frequency. The tapping mode of operation combines qualities of both the contact and non-contact modes by gleaning sample data and oscillating the cantilever tip at or near its natural resonance frequency while allowing the cantilever tip to impact the target sample for a minimal amount of time these micro-cantilever [6].

Thus, dynamic analysis of this kind of instrument is a significant and important task, especially in the tapping mode. Identifying the tip-sample interaction forces makes a crucial role in dynamic analysis and application of AFM, and is studied herein. These forces have a highly nonlinear behavior depending on a number of factors, such as different materials properties, different surface forces, operating conditions, etc., which affect the separation-amplitude relation. These phenomena make the important problem of identifying different surface forces quite challenging [7]. For small tip–sample distances (less than a nanometer), the tip–sample interaction can be large enough so that a nonlinear dynamical behavior of the oscillating system happens. The nonlinear behavior of the oscillator makes the description of the experiment more difficult to predict, but in turn the nonlinear behavior induces a high sensitivity of the oscillator in the proximity the surface that produces images with a nanometer scale contrast [8]. Figure (1) shows a schematic of AFM.

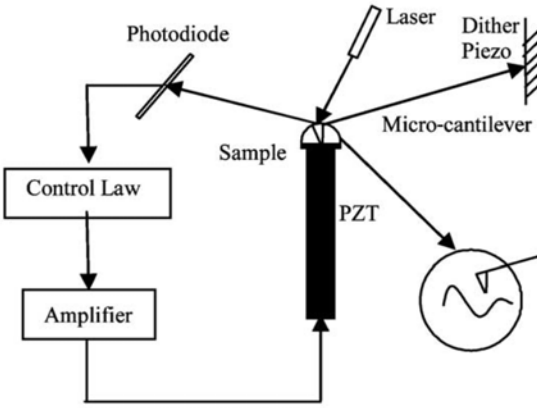

Fig. 1 Schematic of basic AFM operation [1]

The forces relevant to AFM are ultimately of electromagnetic origin. However, different intermolecular, surface and macroscopic effects give rise to interactions with distinctive distance dependencies. In the absence of external fields, the dominant forces are van der Waals interactions, short-range repulsive interactions, adhesion and capillary forces [9]. Existence of such forces makes the dynamic behavior of the system more complicated. Winkler et al. [10] ignored long-range interaction forces, for further simplification of calculations. They also considered short-range contact forces described by a harmonic potential. On the other hand, Anczykowski et al. [11] used the sophisticated Muller-Yushchenko-Derjaguin/Burgess-Hughes-White (MYD/BHW) model to calculate tip-surface interaction forces. Moreover, in [12], computer simulations are presented based on BCP (Burnham–Colton–Pollock) contact mechanics and van der Waals surface forces. To present a compromise between a realistic description of the tip-surface interaction and reasonable computational model, some other models are developed. The most popular models are known as Derjaguin-Muller-Toporov (DMT) and Johnson-Kendall-Roberts (JKR), which model the tip-sample interaction forces [13, 14].

2. Interaction forces

In this section, the interaction forces in tapping mode atomic force microscopy are presented.

2.1. Long-range attractive interactions

Long-range interactions of van der Waals type arise from electromagnetic field fluctuations. Field fluctuations are universal which makes van der Waals forces ever-present, independent of the chemical composition of the surfaces or the medium. Van der Waals forces are amenable to several theoretical treatments of varying complexity. However, simple approximations are usually used for a geometry (sphere-flat) that resembles the tip-surface interface [9].

2.1.1. Van der Waals force

Assuming that the tip-sample geometry could be modeled by a sphere (tip apex) in the vicinity of a flat surface (the sample), the van der Waals force, F_{vdW} , can be written as [15]:

$$F_{vdW}(d)=\begin{cases}-\dfrac{HR}{6d^2} & d>a_0\\ -\dfrac{HR}{6a_0^2} & d\le a_0\end{cases} \tag{2.1}$$

In the above relation, H is the Hamaker constant, R is the tip radius, and d is the instantaneous tip-sample separation distance. The parameter a_0 is the intermolecular distance which is introduced when $d\rightarrow 0$ to prevent the divergence of the van der Waals force. As equation (2.1) indicates, at distances shorter than a_0, it is assumed that the van der Waals force is constant and equal to its magnitude at $d=a_0$.

2.2. Contact and short-range repulsive forces

Repulsive forces between atoms or molecules arise from Pauli and ionic repulsion. However, if the contact area between two objects involves tens or hundreds of atoms, the description of the effective repulsive force can be obtained without considering Pauli and ionic repulsion. The surfaces of two bodies are deformed when they are brought into mechanical contact. The deformation depends on the applied load and the properties of the material. Continuum elasticity theories describe the contact and adhesion between finite bodies under an external load [9]. Theories for deformable spheres were presented by Derjaguin et al. [16] as DMT model and by Johnson et al. [17] as JKR model. Furthermore, to present the intermediate regime between JKR and DMT models, Maugis-Dugdale (MD) formulation is developed in [18]. In this theory, the surface force is assumed to be a constant up to a maximum separation beyond which it falls to zero. Johnson and Greenwood [19] presented an adhesion map for the contact of elastic spheres.

2.2.1. DMT model

For describing stiff contacts with low-magnitude adhesion forces and small tip radii, the DMT model is appropriate [16], [20]. In this model, the repulsive contact force, F_{rep}^{DMT}, is calculated from the following equations:

$$F_{rep}^{DMT}(d)=\frac{4}{3}E^{*}\sqrt{R}\left(a_0-d\right)^{3/2}$$
$$\frac{1}{E^{*}}=\frac{1-\nu_t^2}{E_t}+\frac{1-\nu_s^2}{E_s} \tag{2.2}$$

where E^{*} is the effective elastic modulus, E is the elastic modulus, and ν is the Poisson's ratio. The subscripts $''t''$ and $''s''$ refer to the tip and sample, respectively. Also, the adhesion force, F_a^{DMT}, is defined as:

$$F_a^{DMT}=-4\pi R\gamma=-\frac{HR}{6a_0^2} \tag{2.3}$$

where γ is the surface energy. The relations related to the contact radius *(a)* and deformation *(δ)* are as follows:

$$a=\left(\frac{R\left(F_{DMT}-F_a^{DMT}\right)}{K}\right)^{1/3},\quad \delta=\frac{a^2}{R}\quad,\quad K=\frac{4}{3}E^{*} \tag{2.4}$$

F_{DMT} is the tip-sample interaction force (including the repulsive and the adhesion contact forces) for the distance range of $d\le a_0$, which can be used in appropriate relevant conditions.

2.2.2. JKR model

The JKR model should be selected for relatively low-stiff contacts with high-magnitude adhesion forces and large tip radii [17], [20]. In this model, the adhesion force, F_a^{JKR}, is estimated as follows:

$$F_a^{JKR}=-3\pi R\gamma=-\frac{9}{8}\frac{HR}{6a_0^2} \tag{2.5}$$

The following relation shows the association of the contact radius (a) with the applied (loading) force, F_{JKR}.

$$a=\left(\frac{R}{K}\right)^{1/3}\left(\sqrt{-F_a^{JKR}}\pm\sqrt{F_{JKR}-F_a^{JKR}}\right)^{2/3} \tag{2.6}$$

The negative sign indicates unstable conditions. The resulting deformation (δ) could be estimated through the following relation:

$$\delta = \frac{a^2}{R} - \sqrt{\frac{16\pi\gamma a}{3K}} \tag{2.7}$$

2.2.3. Capillary forces

In ambient conditions, a thin film of water is adsorbed on hydrophilic surfaces. At close proximity of tip and surface, the separation scales with the Kelvin radius, a meniscus or liquid bridge may be formed between tip and sample. This meniscus implies an attractive (capillary) force that shows a dependence with the distance [9]. The distances at which this liquid bridge forms ($d=d_{on}$) or breaks ($d=d_{off}$) are totally different, and this behavior causes the capillary force to become hysteretic. In the simple model presented by Zitzler et al. [15] for the capillary force, these distances are determined in the following way:

$$\begin{cases} d_{on} = 2h \\ d_{off} = V_{men}^{1/3} - \frac{1}{5R} V_{men}^{2/3} \end{cases} \tag{2.8}$$

In the above relation, h is the thickness of the water film. Here, the thicknesses of the water films on the tip and sample are assumed to be the same. V_{men} is the meniscus volume between the tip and sample which is calculated from the following relation:

$$V_{men} = 4\pi R h^2 + \frac{4}{3}\pi h^3 + 2\pi r^2 h \tag{2.9}$$

r is the radius of the circular contact region between the tip and sample. Applying the DMT theory, and under negligible loading condition, the radius of the contact area is obtained as:

$$r = \sqrt[3]{\frac{3\pi\gamma_{sv} R^2}{E^*}} \tag{2.10}$$

where γ_{sv} is the solid-vapor interfacial energy for both the tip and sample. During the formation of the meniscus, the capillary force can be calculated from the following relation:

$$F_{cap}(d) = \begin{cases} -\frac{4\pi\gamma_{H_2O} R}{1 + d/h} & d > a_0 \\ -\frac{4\pi\gamma_{H_2O} R}{1 + a_0/h} & d \le a_0 \end{cases} \tag{2.11}$$

γ_{H_2O} is the liquid-vapor interfacial energy of water. For simplicity, the magnitude of F_{cap} is assumed as constant at distances less than a_0. The effect of this force is considered by some authors in tapping mode of AFM [21, 22].

The overall tip-sample interaction force F_{ts} is obtained by adding up all the contributing components:

$$F_{ts}(d) = F_{vdW} + F_{(DMT \quad OR \quad JKR)} + F_{cap} \tag{2.12}$$

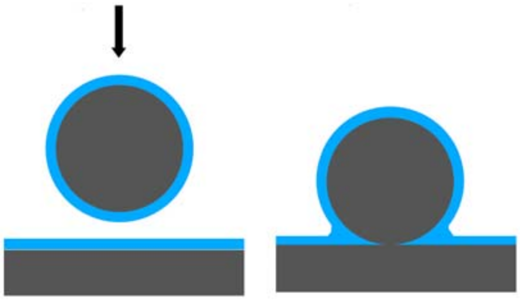

Fig. 2 A schematic of an AFM tip oscillating above a sample in ambient conditions [21]

3. Roughness effect on contact mechanics models

Rabinovich et al. [23] took into account both height and breadth of asperities motivated by the availability of AFM. They employed root mean square roughness which can easily be determined by AFM surface imaging, to describe the asperities. They also advanced the model with two scales of roughness in order to provide an accurate description of the surfaces on the nanoscale [24].

The Rumpf–Rabinovich formulation is widely regarded as the most accurate model to predict interparticle van der Waals adhesion for materials with a rough surface. However, it suffers the serious shortcoming in that the local deformations of the contacting surfaces are entirely neglected [25]. All these approaches use mean adhesion forces. Li et al. [26] combined JKR and DMT models considering Rumpf – Rabinovich roughness model.

As almost all of the surfaces in reality are not really flat or smooth, the van-der-Waal equation became adapted to rough surfaces by calculating the roughness as a half sphere (radius r) with its centre on top of the surface (Rumpf) and with its centre beneath the surface [27]:

$$F_{vdw} = \frac{Hd}{12a^2}\left[\frac{1}{1+\frac{d}{2r}} + \frac{1}{\left(1+\frac{r}{a}\right)^2}\right] \tag{3.1}$$

where H is the surface material, d is particle diameter, and r is roughness parameter. By varying just one of these parameters wile the others are kept constant, the influence of each parameter can be detected. According to Eq. (3-1) the dependence of the van der Waal force on the particle diameter and the roughness radius is shown in Fig. 3.

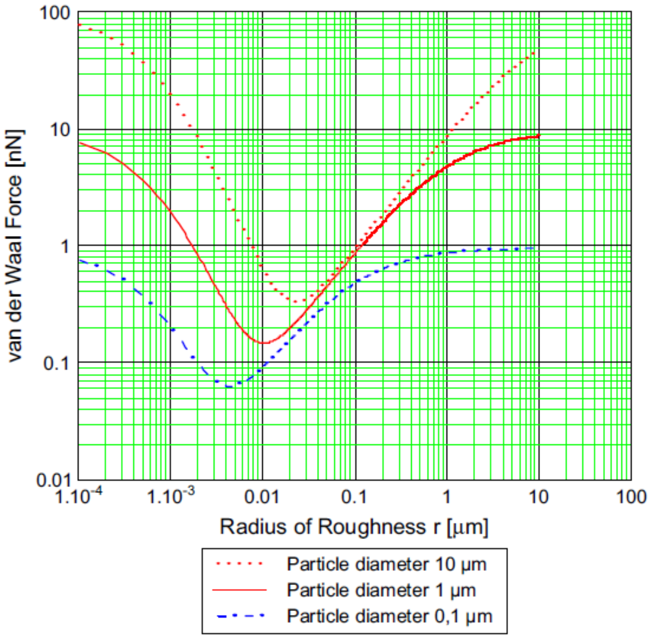

Fig. 3 Dependence of van der Waal force on the roughness radius [27]

4. Conclusions

To develop the application of tapping mode atomic force microscopy, one must have a correct understanding of the tip-sample interaction forces, especially for high-precision images and reliable data in nanoscale. Thus, identifying the tip-sample interaction forces which are effective in performance of the system will result in a proper analysis of AFM dynamics, and accordingly selecting the appropriate operating conditions. In this research, a review has been presented on tip-sample interaction forces in tapping mode atomic force microscopy. The forces have been categorized into long-rage and short-range ones. The Van der Waals forces have been introduced as the long-range ones, and the contact forces presented as the short-range ones. Some important models such as DMT and JKR have been studied as the nano-contact mechanics models to develop the contact forces. Moreover, the capillary forces and roughness effects have been studied in this paper.

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