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Nanomanipulation Modeling and Simulation

by

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Abstract

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A novel approach to better model nanomanipulation of a nanosphere lying on a stage via a pushing scheme is presented. Besides its amenability to nonlinear analysis and simulation, the proposed model is also effective in reproducing experimental behavior commonly observed during AFM-type nanomanipulation. The proposed nanomanipulation model consists of integrated subsystems that consistently define the dynamics of the nanomanipulator tip and nanosphere, friction between the nanosphere and the stage, and the contact deformation between the nanomanipulator tip and the nanosphere. The main feature of the proposed nanomanipulation model is the Lund-Grenoble (*LuGre*) dynamic friction model that reliably represents the stick-slip behavior of atomic friction experienced by the nanosphere. The *LuGre* friction model introduces a new friction state and has desirable mathematical properties making it a well-posed dynamical model that characterizes friction with fidelity. The proposed nanomanipulation model facilitates further improvement and extension of each subsystem to accommodate other physical phenomena that characterize the physics and mechanics of nanomanipulation. Finally, the proposed model is simulated and compared to existing modes in the literature to demonstrate its versatility and effectiveness.

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Chapter 1

Introduction

Nowadays, researchers have narrowed their research focus down to the nanometer dimension that is referred as nano level. One particular interest is to develop nanotechnology that creates a macroscopic structure having a carefully controlled arrangement in the nano scale. The electronic industry in particular will reap great benefits from the development of nanotechnology. Powerful computers with faster processors and larger data storage capacity will no longer be out of reach in the near future [63]. One way to achieve fabrication of nano-scale components is by direct force manipulation of objects such as carbon nanotubes, silicon whiskers, nanowires, nanoshells, polymer particles and biological molecules using nano probes (tips). Several research groups have reported precise manipulation of nanoparticles to form two or even three dimensional patterns with appropriate chemical or thermal processes [51, 41, 35]. This force-based nanomanipulation could be achieved for example by employing Scanning Tunneling Microscopy (STM) [3], Atomic Force Microscopy (AFM) [24, 22], or by a recently developed nanomanipulator manufactured by Zyvex [77].

Basically, STM and AFM are imaging devices for nano objects. The invention of STM and AFM in past two decades has enabled scientists and engineers to extend their studies to objects at the atomic level. Many structures and properties of such objects have been obtained by these microscopes. The following section briefly presents the underlying principles of STM and AFM operations that have revolutionized the modern study of atomic particles. The subsequent section discusses the available nanomanipulators that are chiefly derived from the imaging devices. The description of the considered nanomanipulation and the motivation of modeling such a system will be given in the final section.

1.1 STM and AFM Imaging Principles

Scanning Tunneling Microscopy (STM) makes use of the quantum electron tunneling principle to attain its functionality. The STM operation can be thought of as an open circuit having a voltage source. The gap between the tip and the conducting sample is the potential barrier. The circuit is open when the gap is sufficiently large. This large gap suppresses the tunneling probability of electrons to zero. As the tip is brought closer to the sample surface, the tunneling probability increases which means that a higher percentage of current flows across the circuit. The properties of the sample can then be inferred from the the gap size and the amount of current flowing for a given electrical potential at a particular plane coordinate.

Unlike STM that uses the quantum tunneling principle, Atomic Force Microscopy (AFM) utilizes a classical mechanics approach. The free end of the AFM tip will deflect in the direction of applied force. For a small deflection, the force-deflection relationship obeys the Hooke's law:

$$F = k\delta \tag{1.1}$$

where F is the induced force; k is the Hooke's proportionality constant; δ is the deflection of the cantilever tip.

As the AFM tip approaches or even touches and exerts a force on the sample surface, the tip will deflect accordingly either due to the tip-sample interaction force or because of the force repercussion from the exerted force on the sample surface. Hence, the properties of the sample can be deduced from the amount of deflection and the inherent material properties of the AFM at a particular plane coordinate.

1.2 Nanomanipulators

A nanomanipulator is a robot that can manipulate objects in nanometer size (nano objects) with nanometer precision [61]. Nanotubes and nanoparticles are examples of nano objects. An ideal nanoparticle is a spherical nano object with a diameter less than a micrometer [63, 62]. Although AFM and STM were originally intended to be atomic imaging instruments, they can be nanomanipulation tools as well. Zyvex S100 system is another example of nanomanipulator [77]. The corresponding manipulation

method of each nanomanipulator will be discussed in this section. The advantages and disadvantages of the nanomanipulators will also be compared against one another.

AFM nanomanipulation makes use of a sharp cantilever tip to drag a sample across the stage. The tip has to have a sufficient spring constant and needs to overcome the tip-sample force interaction to be able to achieve its manipulation objective. In STM nanomanipulation, a regulated current is tunneled from the tip to the conducting sample or vice versa [60] to give a desired lifting force to the object. Manipulation of the object can be achieved by two methods. The first method is to completely lift the object and have it deposited in another place [20]. The second method is to drag the object across the sample holder while maintaining enough attractive force between the tip and the object [46]. The Zyvex S100 system has four probes mounted horizontally in plane each at 90° angle. The probe cross-section can be either rectangular or tubular with a tapered conical tip. Similar to STM, the S100 system with the correct coordination of the four probes is also able to do pick and place operation in manipulating the object.

In comparison, STM has a better sensitivity than AFM and the Zyvex nanotips because STM operates in the region where the tunneling current varies exponentially with small tip-sample separation distance as illustrated in figure 1.1. On the other hand, the sensitivity of the nanotips is only proportional to the cantilever stiffness [31], [6].

But, STM suffers from the fact that it requires the sample to be electrically conductive. On the other hand, AFM and the Zyvex S100 systems can deal with any kind of materials without requiring electrical conductivity property.

Figure 1.1: STM and AFM operating region

STM manipulation may also need to be conducted in vacuum to avoid solid surface changes due to adsorption and desorption of atoms and molecules [31, 55]. The unwanted impurities on the surface will pose as barriers to the manipulation via dragging method. Another potential problem is surface inhomogeneity, which causes variations of electrical conductivity in different regions [46]. Hence, the inhomogeneous surface affects the attractive strength between the tip and the sample that facilitates the pulling mechanism to the sample as the STM tip moves across the sample stage.

Due to its inability to image the sample topography, the S100 system also needs to be integrated with a visual sensor such as Scanning Electron Microscopy (SEM). This deficiency renders the entire S100 manipulation inoperable in ambient conditions. On the other hand, AFM can function in both ambient and vacuum environments.

This work considers modeling of nanomanipulators such as AFM and the Zyvex devices that can accommodate manipulation of nano objects that are not electrically conductive.

1.3 Motivation and Outline of the Thesis

Since the manipulated sample experiences complex interactions with the tip and the stage, modeling of the nanomanipulation is crucial in understanding the physics behind the process [34]. Recently, friction between the sample and the stage has sparked interest among many groups. Baterls et al. conducted STM based nanomanipulations of single atoms [3]. The manipulation was in constant current mode where the change in tip deflection can be recorded to further extract friction data. Falvo et al. used AFM based nanomanipulation to measure friction data of multiwall carbon nanotubes with a diameter of about 30 nm [24, 22]. Sitti also used an AFM based nanomanipulation to push nanoparticles of about a micron size [63, 62]. Experimental data collected in the above mentioned references and others exhibit a stick-slip motion behavior of the sample during the manipulation process [24, 8].

Researchers have proposed models for the AFM based pushing manipulation [70, 69, 75]. Most of these models manage to represent steady sliding of the manipulated object that is commonly observed in macromanipulation. They are not able, however, to reproduce the stick-slip characteristic of nano friction. This is mainly due to the use of conventional static friction models such as Coulomb fric-

tion and discretized friction cone models. Although some other researchers manage to construct continuous static friction models that explain nano friction phenomena [45, 53, 68], static friction models still have inherent shortcomings such as the inability to account for the presliding condition [47], the improper assumption of rapid relaxation processes in the lubrication film [48], and the undesired creeping sample movement under a nonzero external force.

The existing AFM manipulation models either impose a very restrictive condition or make use of momentum analysis to address the collision process of the tip and the sample. But, those approaches are ineffective in describing the complete collision process that may be of interest in studying other possible dynamic contact deformation profiles. The dynamic model in [70, 69], does not explain the collision impact between the tip and the sample because of the assumption of a constant contact deformation between the tip and the sample during the manipulation process. Despite the introduction of momentum analysis along with the coefficient of restitution to help estimate the resulting impulse magnitude, the model in [75] remains unable to describe the transient collision process as well. Moreover, both Coulomb switching and momentum analysis approaches require an accurate (and computationally expensive) zero-crossing detection to be well-implemented in a numerical simulator.

This work presents a comprehensive and practical model of a nanotip-based nanomanipulation that improves existing micro/nano manipulation models in the literature. Figure 1.2 illustrates how unidirectional nanomanipulation could be achieved using

for example an AFM or using only one nanotip of the Zyvex nanomanipulator. The nanoparticle is strongly adhered to the stage surface by the sample–stage interaction force. The motion of the tip is responsible for manipulating the nanoparticle to a new position on the stage surface. A sufficient spring stiffness of the tip is required to overcome the tip–sample interaction forces in dragging a nanoparticle across the stage. The tip diameter needs to be smaller than the diameter of the nanoparticle so that the tip can be controlled to push the nanoparticle without touching the stage. State of the art technologies enable the production of sharp AFM and the Zyvex tips that have a radius of 5 nm [77]. Nonetheless, there is no guarantee that defects such as contamination and misshapen tips will never occur. Both contamination and misshapen tips may occur either during the manufacturing process or during the imaging process [73].

Figure 1.2: Schematic of one axis AFM and Zyvex nanomanipulation (not to scale)

The proposed model encompasses physics and mechanics of the nanomanipulation. The model consists of inter-related modules that describe interaction forces and contact deformation between the tip and the sample, the tip and sample dynamics, and friction on the sample-stage interface. The development of the modules is based on the utilization and extension of previous work found in the literature. The schematic of the modular interconnect of the proposed manipulation model is illustrated in Figure 1.3.

Figure 1.3: Modular Interconnect of the proposed AFM manipulation model

The remainder of the thesis is organized as follows. The cantilever and its components will be modeled as lumped systems in Chapter 2. The sample is assumed to be an elastic perfect sphere (i.e. a nanosphere) and is also modeled in Chapter 2. Interaction forces that may arise in the atomic level are discussed in Chapter 3. The resulting deformation of both the tip and the sample during the nanomanipulation will be analyzed by a continuum contact mechanics model that is presented in Chap-

ter 3 as well. Chapter 4 presents a dynamical friction model to describe the friction on the sample-stage interface. Once the model has each module completely described, simulations of the proposed nanomanipulation model with varied parameters are presented to capture the dynamic characteristics of the model in Chapter 5. Finally, the thesis ends with conclusions in Chapter 6.

Chapter 2

Nanotip and Sample Dynamics Models

Mechanical systems are examples of dynamical systems rigorously studied by scientists and engineers. The modeling of mechanical systems mostly follows a systematic procedure that utilizes Newton's Laws. This chapter focuses on dynamics modeling of a nanotip and a spherical sample to be manipulated. The resulting model only accounts for the single-degree of freedom (SDOF) pushing dynamics of the nanotip. The SDOF model is perfectly suited to describe the dynamics modeling of the Zyvex nanomanipulator that utilizes its single nanotip. The model also applies to the AFM nanotip if the AFM base cantilever is assumed to be rigid as illustrated in Figure 1.2.

The resulting dynamics models will represent the nanotip and sample modules of the nanomanipulation model as illustrated in Figure 1.3. Various approaches to model the AFM cantilever either as a continuous or a point mass system will first be briefly discussed. The subsequent section will propose lumped mass modeling of the nanotip. Finally, the dynamics model of the sample will be presented in the last section.

2.1 Literature Review

There are two major models used to represent the AFM cantilever, both being in the form of differential equations. Both dynamical models assume a linear operating region meaning that the validity of the models is in a small perturbation area about the equilibrium.

The first dynamical model, also known as the distributed parameter model, treats the cantilever as a continuous system. The distributed parameter model is represented by partial differential equations. External forces acting on the cantilever are prescribed in the appropriate boundary conditions [50, 52]. In this model, the deflection of each continuous axial element of the cantilever can be calculated by solving the differential equations. Rahman characterizes the contact stiffness of surfaces (to tell if it is Hertzian or not) using the AFM in tapping mode [50]. The cantilever along with the restoring force by the surface at the point of contact are modeled by the first dynamical model and a third order polynomial function, respectively. The coefficients of the polynomial function are inferred from Hertzian contact theory. The characterization approach is to use the perturbation method (up to sufficient number of modes) to solve the derived differential equations. The numerical results show that a softer contact, which is not Hertzian, will yield a lower cantilever vibration amplitude that exhibits in the cantilever's first mode response. As another example, Sader uses the distributed parameter model to develop a theoretical model for the frequency response of an AFM cantilever beam that is immersed in a viscous fluid and excited

by Brownian thermal motion [52]. As a final example, Stark creatively represents an AFM cantilever in response to the tip-sample interaction as a linear time-invariant system in state space with nonlinear output feedback [66]. The state space representation is directly derived from the first dynamical model via the so-called modal analysis and mode-summation method.

On the other hand, the second dynamical model considers the cantilever as a point mass having properties directly derived from the distributed parameter model. The full solution to the partial differential equations of the distributed parameter model is redundant if the deflection of the cantilever tip is the main part of the cantilever to analyze. External forces are formulated directly acting on the point mass. Unlike partial differential equations of continuum mass, ordinary differential equations do not involve boundary conditions and only deal with discrete objects. Therefore, many researchers prefer to approximate the cantilever as a discretized point mass using the second dynamical model [2, 9, 59, 58, 54]. Here, the point mass can be thought of as a corresponding lumped mass at the cantilever tip. Generally, the second dynamical model or the lumped mass model approximates the distributed parameter model only up to its first natural frequency assuming that the cantilever is not vibrated exceeding its first resonance. The effective mass and stiffness that are used in the lumped mass model can be inferred directly by equating corresponding natural frequencies of both the distributed parameter model and the lumped mass model. Nevertheless, in imaging operation via tapping mode for instance, the AFM cantilever needs to

be vibrated as fast as possible to minimize the time to acquire the sample image and to obtain a better image resolution. In that case, the oscillation frequency often exceeds the first natural frequency of the cantilever. Although the distributed parameter model, which theoretically can account for infinite natural frequencies, seems to be the only suitable model, the lumped mass model will also qualify by utilizing sufficient vibration modes of corresponding natural frequencies [49]. Ashhab analyzes the phase portrait of a micro cantilever in response to attractive van der Waals force [2]. The micro cantilever is represented by the lumped mass model. The resulting phase portrait reveals a homoclinic loop having a fixed point and centers inside the loop. The fixed point represents a gap between the sample surface and the cantilever tip where the tip is in equilibrium. A critical fixed point (a saddle point) is located at the intersection of the stable and unstable manifolds. Since the system is Hamiltonian, all of the trajectories starting inside the loop are stable. Other trajectories that start outside the homoclinic loop are unstable because they eventually hit the sample surface and equilibrate with the sample surface assuming that the surface is soft enough to dissipate energy from the resulting collision. As another example, Sebastian uses the lumped mass model with additional negative and positive springs representing the attractive and repulsive interaction forces, respectively, to model the AFM operation in tapping mode [59, 58]. The model manages to re-create the “jumping” phenomenon that occurs when the vibrating cantilever tip is brought closed to a sample surface. The jumping phenomenon is because of the attractive van der Waals

force between the cantilever tip and the sample surface that pulls the tip toward the sample surface. During the jumping process, the cantilever tip undergoes a softening cantilever stiffness. As a final example, Salapaka models the AFM friction imaging using the lumped mass model as well as the generalized “continuous” Coulomb friction model that is derived from the Johnson - Kendall - Roberts (JKR) theory (a continuum contact theory) [54]. In this case, the lumped mass model also facilitates a control law design for tracking purposes.

Besides the two major models for the AFM cantilever, there is another known approach, which is a hybrid model. Tafazzoli uses the hybrid approach that combines the rigid body formulation for the AFM tip and continuous vibration model to calculate the cantilever’s effective stiffness [70]. Unfortunately, the validity of the hybrid model becomes questionable because of the rigid body formulation and the modeling inconsistency. As an example, the first bending natural frequency of the AFM tip with a uniform cross section obtained from the continuous model [43] is approximately $\omega_{n,1} = \sqrt{\frac{1.875^4}{3} \frac{3EI}{mL^3}}$. On the other hand, Tafazzoli’s rigid body model gives an underestimated natural frequency of $\omega_n = \sqrt{\frac{3EI}{mL^3}}$.

Among the mentioned AFM imaging models, Salapaka’s friction imaging model [54] is the only example of AFM contact mode modeling. The friction imaging model resembles the proposed nanomanipulation model. Differences between the two models are summarized as follows. Salapaka’s friction imaging model deals with the interaction between the cantilever tip and the surface profile. The imaging model also

accounts for the adhesion effect between the tip and the surface. The topography of the surface is provided by an external input of surface profile. On the other hand, the proposed nanomanipulation model considers the interaction between the cantilever tip and the sample that is deposited on top of a layered stage. The interaction forces are assumed to be the attractive van der Waals force and the repulsive force due to possible contact deformation of both the tip and the sample. The topography of the stage surface can be further inferred from the tip-sample interaction forces during the manipulation process.

2.2 Nanotip Dynamics

In this section, a lumped mass dynamical model will be used to represent the possible bending displacements of the nanotip. The parameters of the lumped mass model will first be determined from its corresponding unforced distributed parameter model. Once the corresponding parameters have been derived, the proposed lumped mass models will be presented.

2.2.1 Unforced Distributed Parameter Model

In this model, the nanotip is treated as a continuous system interacting with the sample on its free end. Unlike the lumped mass model, the distributed parameter model theoretically considers infinite harmonics of the cantilever vibrations. The first harmonic of the unforced distributed parameter model for the bending mode is

derived to determine the effective mass that can be used in the free lumped bending vibration of the cantilever [43]:

$$M(x, t) = EI(x) \frac{\partial^2 y(x, t)}{\partial x^2} \quad (2.1)$$

$$\frac{\partial^2 M(x, t)}{\partial x^2} dx = -m_x(x) dx \frac{\partial^2 y(x, t)}{\partial t^2} \quad (2.2)$$

by substituting eq. (2.1) to eq. (2.2), the resulting equation of motion is as follows:

$$\frac{\partial^2}{\partial x^2} \left[EI(x) \frac{\partial^2 y(x, t)}{\partial x^2} \right] = -m_x(x) \frac{\partial^2 y(x, t)}{\partial t^2} \quad (2.3)$$

where E = the cantilever elastic moduli

$I(x)$ = the cantilever area moment inertia

$m_x(x)$ = the cantilever mass per unit length

$$\text{Initial conditions} = \begin{cases} y(x, 0) = y_0(x) \\ \dot{y}(x, 0) = \dot{y}_0(x) \end{cases}$$

$$\text{Boundary conditions} = \begin{cases} y(0, t) = 0 \\ y'(0, t) = 0 \\ y''(L, t) = 0 \\ y'''(L, t) = 0 \end{cases}$$

The method of separation of variables is used to solve eq. (2.3). The first harmonic of the vibration for a bar with a uniform cross section is found to be [43]:

$$\omega_{n,1} = \sqrt{\frac{1.875^4}{3} \frac{3EI}{(m_x L) L^3}} = \sqrt{\frac{1.875^4}{3} \frac{3EI}{m L^3}} \quad (2.4)$$

where $k_{y,e} = \frac{3EI}{L^3}$ or $\frac{2EI}{L^3}$ the cantilever effective bending spring stiffness

due to normal force and bending moment, respectively.

$$m_{y,e} = \left(\frac{3}{1.875^4}\right) m \text{ or } \left(\frac{2}{1.875^4}\right) m \quad \text{the cantilever effective bending mass}$$

due to normal force and bending moment, respectively.

In general, the clamped-free uniform cantilever has the following bending mode shape

$Y(x)$ [71]:

$$\begin{aligned} Y(x) &= \sum_{r=1}^{\infty} Y_r(x) = \sum_{r=1}^{\infty} B[(\cos \beta_r x - \cosh \beta_r x) \\ &\quad - R(\sin \beta_r x - \sinh \beta_r x)] \end{aligned} \quad (2.5)$$

$$\begin{aligned} \text{where } \beta_r^4 &= \frac{\omega_{n,r}^2 m_x}{EI} \\ R &= \frac{\cosh \beta_r L + \cos \beta_r L}{\sinh \beta_r L + \sin \beta_r L} \end{aligned}$$

that satisfies the following condition:

$$\cosh \beta_r L \cos \beta_r L + 1 = 0 \quad (2.6)$$

Rayleigh's energy method may also be used to obtain an estimate of the first natural frequency [33]. The method facilitates the first natural frequency estimate of a system with varying cross sectional area, density, and elastic moduli. The method for a bending vibration is as follows [43]:

$$E = 0 + T_{\max} = V_{\max} + 0 \quad (2.7)$$

$$T_{\max} = V_{\max}$$

$$\begin{aligned} \text{where} \quad T(t) &= \frac{1}{2} \int_0^L m_x(x) \left[\frac{\partial y(x,t)}{\partial t} \right]^2 dx \\ V(t) &= \frac{1}{2} \int_0^L EI(x) \left[\frac{\partial^2 y(x,t)}{\partial x^2} \right]^2 dx \\ A(x) &= \text{cross sectional area of the cantilever} \end{aligned}$$

$$\text{let} \quad y(x,t) = Y(x)f(t) \quad (2.8)$$

$$\begin{aligned} \text{then} \quad T(t) &= \frac{1}{2} \dot{f}^2 \int_0^L m_x(x) Y^2(x) dx \\ V(t) &= \frac{1}{2} f^2(t) \int_0^L EI(x) \left[\frac{d^2 Y(x)}{dx^2} \right]^2 dx \\ \omega_n^2 &= \frac{V_{\max}}{T^*} = \frac{\int_0^L EI(x) \left[\frac{d^2 Y(x)}{dx^2} \right]^2 dx}{\int_0^L m_x(x) Y^2(x) dx} \end{aligned} \quad (2.9)$$

2.2.2 Lumped Mass Model

This section presents the dynamics modeling of the nanotip module of the nanomanipulation model. The nanotip is treated as a point mass interacting with the sample. The modeling will use the lumped mass model that only considers the first vibration mode of the corresponding distributed parameter model. The parameters

of the lumped mass model are derived from the corresponding distributed parameter model in the previous subsection. The lumped mass models are valid if the cantilever operates in the frequency region that is less than its first natural frequency. The assumption of a small deflection is also implicit in the proposed lumped mass model.

Figure 2.1: Tip-sample coordinates

Figure 2.1 shows coordinates of the tip y_t and of the sample y_s that correspond to the setup illustrated in Figure 1.2. The tip-separation distance $\tilde{y}$ is defined as the position difference between the outermost atoms of the tip and the sample:

$$\tilde{y}(t) = y_s(t) - (R_{\text{sample}} + R_{\text{tip}}) \quad (2.10)$$

Assuming that the stiffness of the tip is higher than that of the sample, it is reasonable to represent the dynamics of the nanomanipulation tip with a single degree of freedom (SDOF) lumped parameter dynamic model [72, 9]. The axial balance of

forces on the tip along the pushing axis y_t results in the following equations:

$$\begin{aligned}
m_t \ddot{y}_t(t) + c_t \dot{y}_t(t) + k_t y_t(t) &= c_t \dot{y}_b + k_t y_b(t) - F_{ts} & (2.11) \\
m_t &= \frac{3\rho_{\text{tip}} A_t L_t}{(1.875)^4} \\
k_t &= \frac{3E_t I_t}{L_t^3}
\end{aligned}$$

where m_t is the tip effective mass, k_t is the tip effective stiffness, c_t is the tip damping coefficient, $y_b(t)$ and $y_t(t)$ are the tip base and the actual lateral tip movements respectively, $\dot{y}_b$ is a constant tip base velocity, E_t is the tip elastic modulus, A_t is the tip cross sectional area, I_t is the tip moment of inertia, L_t is the length of the tip, and ρ_{tip} is the tip material density. F_{ts} is the lateral tip-sample interaction forces defined in the next chapter.

2.3 Sample Dynamics

The dynamics formulation for the sample will be presented in this section. The sample is assumed to be an elastic spherical object situated on a stage. Newton's Laws will be used to derive the equation of motion of the sample. Besides friction, the sample will experience sample-stage and tip-sample interaction forces. The sample-stage interaction forces plus the external applied load from the tip determine the friction that the sample will encounter. The tip-sample interaction forces are responsible for coupling the push-pull mechanism to the sample. By balancing all of the forces, the

equations of motion for the sample are given as follows:

$$N_s = F_{ss} + m_s g \quad (2.12)$$

$$m_s \ddot{y}_s(t) = F_{ts}(\tilde{y}) - F_{\text{rict}} \quad (2.13)$$

where N_s is normal force on the sample, F_{ss} is sample-stage interaction forces, g is the gravitational constant, F_{rict} is friction between the sample and the stage that will be modeled in Section 4.14, m_s is sample mass, $F_{ts}(\tilde{y})$ is the tip-sample interaction force defined in Section 3.1.1.

Chapter 3

Interaction Forces and Contact Mechanics

This chapter discusses interaction forces that may arise at the nano level and contact deformation of two contacting objects as a result of a compressive force acting on the contacting surface. The first half of the chapter will deal with interaction forces. Types of interaction forces will be briefly introduced and discussed. The proposed model along with other models of interaction forces will then be presented. A brief introduction of contact deformation and its prior contact modeling approach will also be discussed. The discussion of contact deformation along with the proposed modeling and other contact models will ensue in the remainder of the chapter. The proposed models of interaction forces and contact deformation will represent the tip - sample interaction and contact mechanics modules of the nanomanipulation model as illustrated in Figure 1.3.

3.1 Interaction Forces

In macroscopic body, gravity has a dominant force between two interacting bodies. As the size of the interacting body decreases, intermolecular force becomes more

significant than gravity. Gravitational and intermolecular forces are proportional to the object volume and surface area, respectively [44]. The cubic term of the volume will be larger than the quadratic term of the surface area when the dimension of the object is large enough. This pattern reverses as the object dimension scales down. The gravitational and intermolecular forces are described by two different equations, and their applications are regulated by the object size. To refine the abrupt switching condition of the two equations, researchers have proposed better models to unify the gravitational and intermolecular forces by imposing appropriate constraints as discussed in a paper by Fischbach [25].

This work only considers three major interaction forces that are long-ranged type in the nano level. The forces are capillary, electrostatic, and van der Waals forces. Capillary force arises from the surface tension due to the liquid present in the ambient air. Coulomb and electrical double layer forces constitute the electrostatic interactions. Whereas van der Waals force consists of dipole-dipole (both atomic dipoles are free to rotate), free to rotate dipole-non polar, and non polar-non polar interactions. Those three types of van der Waals interactions are known as Keesom, Debye, and London (dispersion) interaction, respectively. The combination of double layer and van der Waals forces is known as Derjaguin-Landau-Verwey-Overbeek (DLVO) force [55].

Among the mentioned interaction forces, van der Waals force will always be present. The capillary forces can be eliminated if the nanomanipulation is conducted

Figure 3.1: Van der Waals interactions [38]

in a vacuum chamber. The coulomb interaction that is due to charged particles can be removed as well by properly grounding interacting objects. The electrostatic force due to the electrical double layer may still persist between two interacting objects through an aqueous interface because of the adsorption of OH^- or H^+ of dissociated water [55]. However, similar to capillary forces, the electrical double layer can be eliminated as well in a vacuum chamber. In terms of the magnitude, the highest and the lowest contributors are the capillary and the electrostatic forces, respectively [64].

The three types of van der Waals interactions are illustrated in Figure 3.1. The London dispersion interaction is mostly responsible for the entire van der Waals interaction although the Keesom interaction becomes considerable or even greater than the London's in highly polar molecules such as water. Each van der Waals interaction is proportionally related to its corresponding Hamaker's constant. The theoretical

interaction energy of each type of van der Waals force is given below [38]:

$$E_K(r) = -\frac{u_1^2 u_2^2}{3(4\pi\epsilon_0)^2 k T r^6} \quad \text{Keesom Energy} \quad (3.1)$$

$$E_D(r) = -\frac{u^2 \alpha}{(4\pi\epsilon_0)^2 r^6} \quad \text{Debye Energy} \quad (3.2)$$

$$E_L(r) = -\frac{3}{4} \frac{h\nu\alpha^2}{(4\pi\epsilon_0)^2 r^6} \quad \text{London Energy} \quad (3.3)$$

where $\epsilon_0 = 8.854 \times 10^{-12} \left[\frac{C}{V.m} \right]$. is the permittivity constant, $k = 1.38 \times 10^{-23} \left[\frac{J}{K} \right]$ is the Boltzman constant, $h = 6.63 \times 10^{-34} \left[\frac{J}{s} \right]$ is Planck's constant, T is temperature $[K]$; ν is the electronic absorption frequency, α is the polarizability constant, u_n is the dipole moment.

Generally, the van der Waals force between identical molecules across any medium is attractive. On the other hand, dissimilar molecules may experience either attractive or repulsive interaction depending on the nature of the intermediate medium. Commonly, the total van der Waals interaction between two media across a solvent medium (i.e. water) will be lower than the interaction across vacuum. The following Lifshitz theory can help determine the appropriate Hamaker's constant of medium 1 and 2 interaction across medium 3 [38].

$$\begin{aligned} H_{total} &= H_{\nu=0} + H_{\nu>0} \\ &\approx \frac{3}{4} kT \left(\frac{\epsilon_1 - \epsilon_3}{\epsilon_1 + \epsilon_3} \right) \left(\frac{\epsilon_2 - \epsilon_3}{\epsilon_2 + \epsilon_3} \right) \\ &\quad + \frac{3h\nu_e}{8\sqrt{2}} \frac{(n_1^2 - n_3^2)(n_2^2 - n_3^2)}{(n_1^2 + n_3^2)^{1/2}(n_2^2 + n_3^2)^{1/2} [(n_1^2 + n_3^2)^{1/2} + (n_2^2 + n_3^2)^{1/2}]} \end{aligned} \quad (3.4)$$

where ε_n is the static dielectric constants; ν_n is the molecular harmonic frequency; ν_e is the main electronic absorption frequency in the ultraviolet (UV) region; n_n is the medium refractive index in the visible light region; $H_{\nu=0}$ is Hamaker's constant due to Keesom and Debye interactions; $H_{\nu>0}$ is Hamaker's constant due to London dispersion.

For two identical media interaction across a medium, the above equation becomes simplified as [38]:

$$\begin{aligned} H_{total} &= H_{\nu=0} + H_{\nu>0} \\ &\approx \frac{3}{4}kT \left(\frac{\varepsilon_1 - \varepsilon_3}{\varepsilon_1 + \varepsilon_3} \right)^2 + \frac{3h\nu_e}{8\sqrt{2}} \frac{(n_1^2 - n_3^2)^2}{(n_1^2 + n_3^2)^{\frac{3}{2}}} \end{aligned} \quad (3.5)$$

The van der Waals interaction forces as depicted in Figure 3.1 are only valid for an interaction between two atoms. All of individual inter-atomic force interactions have to be considered to define the interaction between objects that are each composed of many atoms (e.g. the interaction between the AFM cantilever tip and the sample). The anisotropy and non-additivity properties of van der Waals force exacerbate the calculations as well. The van der Waals interaction of two atoms is not isolated, but it is the result of other interactions of neighboring atoms.

The van der Waals also has a retardation effect at a considerable separation distance where the interaction decays faster (i.e. from $-\frac{1}{6}$ to $-\frac{1}{7}$) [38]. Theoretically, the retardation effect occurs during the characteristic lifetime of the London force fluctuations when the inter-molecular distance is larger than the distance that light

travels [46]. At such separation distance, the interaction becomes out of phase because by the time the electromagnetic wave of an atom reaches and influences its neighboring atom, the original atomic dipole has changed its orientation. The magnitude of the interaction force then keeps being reduced to zero at an infinite separation distance [27].

For simplicity, the anisotropy, non-additivity, and retardation effect properties of van der Waals interaction will be disregarded. If the entire van der Waals interaction between two atoms/molecules is defined by $V_{\text{vdw}}(z) = -\frac{C}{z^6}$, the resulting force of the interaction is given by $f_{\text{vdw}}(z) = -\nabla V_{\text{vdw}}(z)$. The total force between two interacting objects (assuming constant density on each object) can be the summation of an individual pair interaction of atoms among the two objects [1]:

$$F_{\text{vdw}}(z) = \rho_1 \rho_2 \int_{\forall_1} \int_{\forall_2} f_{\text{vdw}}(z) d\forall_2 d\forall_1.$$

Besides attractive forces, two interacting atoms may experience repulsive forces as they get closer to each other. The repulsion is due to Pauli's exclusion principle saying that no more than two atoms can occupy the same orbit [7]. According to Lennard-Jones potential, the repulsive potential is given by $V_r(z) = \frac{C_r}{z^{12}}$. The combination of both attractive and repulsive potentials will result in the Lennard-Jones potential. A typical Lennard-Jones potential of two interacting atoms is shown in figure 3.2.

The Lennard Jones potential is best suited to describe the interaction of two atoms. Meanwhile, the Derjaguin potential is introduced to represent the interac-

Figure 3.2: Inter-atomic potential energy (Lennard-Jones potential)

tion between two objects having size several times larger than the atomic level. The Derjaguin - Müller - Toporov (DMT) version of the Derjaguin potential [67] can be derived from eq. (3.6) and is illustrated in Figure 3.3.

Figure 3.3: The profile of the Derjaguin interaction force

Note the distinction between the Lennard Johnson and the Derjaguin energy plots that will help us identify the appropriate use of each interaction energy. The Lennard Jones potential has a steeper slope of the energy curve in the repulsive region than the Derjaguin potential. A steeper slope means less deformation of the two interacting objects in the repulsive region. The Lennard Johnson potential also imposes a

vertical asymptote at a given separation distance in accordance to Pauli's principle. On the other hand, the Derjaguin potential relaxes the asymptote to be consistent with possible deformation of contacting objects.

3.1.1 The Proposed Model of Interaction Forces

Surface interaction forces such as meniscus adhesion, electrostatic, and van der Waals forces are present at the nano level. In this work, attractive van der Waals force is expected to be the sole interaction force between the tip and the sample by restricting the nanomanipulation in a clean vacuum chamber with proper electrical grounding. In addition to attractive forces, the tip and the sample may experience a repulsive force as they press against each other that results in a contact deformation. Since the tip and the sample are made of many atoms, the Derjaguin potential is introduced to represent both attractive and repulsive interactions between the tip and the sample. The corresponding Derjaguin interaction force along a pushing axis y is the negative partial derivative of the Derjaguin potential with respect to the pushing axis y : $F_{ts} = -\frac{\partial}{\partial y} V_{\text{DMT}}$ as given below [67].

$$F_{ts}(\tilde{y}(t)) = \begin{cases} -\frac{HR}{6(\tilde{y}(t))^2}, & \text{for } \tilde{y}(t) \geq a_o \\ -\frac{HR}{6a_o^2} + \frac{4}{3}E^*\sqrt{R}(a_o - \tilde{y}(t))^{\frac{3}{2}}, & \text{for } \tilde{y}(t) < a_o \end{cases} \quad (3.6)$$

$$E^* = \left[\frac{1 - v_t^2}{E_t} + \frac{1 - v_s^2}{E_s} \right]^{-1} \quad (3.7)$$

$$\frac{1}{R} = \frac{1}{R_{\text{tip}}} + \frac{1}{R_{\text{sample}}} \quad (3.8)$$

where $\tilde{y}(t)$ is the separation distance between the tip and the sample along the pushing direction, a_o is the inter-atomic separation distance introduced to avoid numerical divergence [30], E^* is the effective tip-sample elastic modulus, R is the reduced tip-sample curvature, v_t and v_s are the Poisson ratio of the tip and the sample, respectively. E_t and E_s are the elastic moduli of the tip and the sample, respectively.

Figure 3.3 sketches the profile of the Derjaguin interaction force. The resulting amount of contact deformation (penetration depth δ) can be directly inferred from the negative amount of the corresponding separation distance $\tilde{y}$ with respect to the inter-atomic separation distance a_o :

$$\delta = -(\tilde{y} - a_o) \quad (3.9)$$

In other words, the initial contact occurs when the outermost atoms of the tip and the sample touch each other. The sign reversal in the penetration depth δ is to enable the application of Hertzian contact mechanics analysis that will be discussed later. In this case, the tip and the sample barely touch each other when the penetration depth δ is equal to zero. Whereas the contact deformation occurs if the penetration depth δ is greater than zero.

3.1.2 Other Models of Interaction Forces

Other interaction force models are available to enhance the simulation of the interaction between the AFM tip and its sample without being restrictive to account

for only van der Waals force. These interaction models can be conveniently incorporated into the proposed module of the interaction forces depending on the nature of nanomanipulation. Some of other interaction models are summarized as follows (note that the negative sign on the equations denote the interaction as attractive):

Adhesion Force between a spherical tip and a flat surface [38]

The following model can accommodate interaction forces such as adhesion, cohesion, capillarity, and surface tension between two interacting objects. Although the model is intended for the interaction between a spherical object and a flat surface, the model can be generalized to account for two interacting spherical objects by appropriately using the effective radius as in eq. (3.8). The complete description of the model is as follows:

$$\begin{aligned}
 F_{adh}(h) &= -4\pi\gamma_{12}R_{tip} \left(1 - \frac{h - 2e}{2r_1} \right) \\
 \gamma_{12} &= \gamma_1 + \gamma_2 - W_{12} \\
 W_{12} &= 2\sqrt{\gamma_1\gamma_2}
 \end{aligned} \tag{3.10}$$

where R_{tip} is the tip radius; γ_{12} is the surface energy between the two interacting objects, W_{12} is the work of adhesion between the sphere and the flat surface, and only applicable to London interaction (neither Keesom nor Debye interactions), h is the tip-sample separation distance, e is the liquid layer thickness, r_1 is the radius of curvature of the meniscus.

Coulombic Force [38]

The electrostatic interactions between two electrically charged objects can be represented as follows:

$$W_{cou}(h) = \frac{Q_1 Q_2}{4\pi\epsilon_0\epsilon h} = \frac{z_1 z_2 e^2}{4\pi\epsilon_0\epsilon h} \quad (3.11)$$

$$F_{cou}(h) = -\frac{dW_{cou}(h)}{dh} = \frac{Q_1 Q_2}{4\pi\epsilon_0\epsilon h^2} = \frac{z_1 z_2 e^2}{4\pi\epsilon_0\epsilon h^2} \quad (3.12)$$

where Q_n is the electric charge of an entity $[C]$, $\epsilon_0 = 8.854 \times 10^{-12} \left[\frac{C}{V.m}\right]$ is the permittivity constant, ϵ is the dielectric constant, $e = 1.6 \times 10^{-19}[C]$ is the electron charge, z_n is ionic valency.

Electrical Double Layer Force [55], [38]

The electrical double layer force due to interaction between low surface potentials through an aqueous medium can be approximated as follows:

$$F_{edl}(d) = \frac{2\zeta_1\zeta_2}{\epsilon_e\epsilon_0} A_c e^{\frac{-d}{\lambda_D}} \quad (3.13)$$

where $\epsilon_0 = 8.854 \times 10^{-12} \left[\frac{C}{V.m}\right]$ is the permittivity constant, ϵ_e is the dielectric constant of the liquid adjacent to the solid, ζ_1 and ζ_2 are the surface charge densities of medium 1 and 2, respectively. λ_D is the thickness of the electrostatic double layer (Debye length).

JKR model [15], [57]

The following model considers both attractive and repulsive interaction forces between two objects that are similar to the proposed DMT interaction force model. The main difference lies in the formulation of those forces. The complete description of the JKR model is as follows:

$$\begin{aligned}
 F_{ts}(z) &= \begin{cases} f_o R \left[-\left(\frac{\sigma}{z}\right)^2 + \frac{1}{30} \left(\frac{\sigma}{z}\right)^8 \right] & \text{for } z > z_o \\ g_o (z_o - z)^{\frac{3}{2}} & \text{for } z \leq z_o \end{cases} \quad (3.14) \\
 g_o &= \frac{8\sqrt{2}}{3\pi \left(\frac{1-v_t^2}{\pi E_t} + \frac{1-v_s^2}{\pi E_s} \right)} \sqrt{R} \\
 f_o &= \frac{2}{3} \pi^2 \epsilon \rho_1 \rho_2 \sigma^4
 \end{aligned}$$

where z is the tip deflection, $z_o = \sigma$ is the separation distance when the Lennard-Jones potential energy is minimum, R is the reduce tip-sample curvature; ρ_i is the atomic/molecular density, ϵ is the minimum energy of the Lennard-Jones Potential, v_t and v_s is the Poisson ratio of the tip and the sample, respectively. E_t and E_s is the elastic moduli of the tip and the sample, respectively.

3.2 Continuum Contact Mechanics

A compressive force induces deformation at the point of contact between two solid objects as they come together. Continuum contact mechanics is a model that

is developed for describing the deformation between the two contacting solid objects. The model is derived from three major theories: elasticity, fracture mechanics, and surface science [55]. The continuum theory assumes the solid object as a continuous medium. On the other hand, an object is physically composed of many atoms. Nevertheless, many experimental data [21, 6], confirm the efficacy of the continuum model to predict the deformation amount at the nano level.

Early work on contact mechanics such as Hertz and DMT models focused on the contact deformation between a spherical sample and a flat surface [16]. This contact mechanics model is applicable to model the contact deformation between the spherical sample and the flat stage. Researchers then generalized the early work to accommodate other contacting object shapes, especially for two contacting spherical objects [16, 38]. This work will particularly consider the developed models for two contacting spherical objects so as to describe the deformation between a spherical tip and a spherical sample during nanomanipulation. The schematics of the contact deformation of sphere - flat objects and sphere - sphere objects are better illustrated in Figure 3.4 and Figure 3.5, respectively.

Figure 3.4: Deformation schematic for sphere-flat surface [55]

According to the figures, the contact deformation is described by the resulting contact radius (a) and contact penetration depth (δ).

Figure 3.5: Schematic of tip-sample contact deformation [38]

Depending on the applicable conditions, the contact models facilitate the inference of contact properties such as the amount of and the area of the contact deformation. The following subsections will first review models of nano contact mechanics and then present the proposed contact model.

3.2.1 Literature Review of Nano Contact Mechanics

In the literature, nano contact mechanics generally embeds interaction forces between two contacting objects into the base model of continuum contact mechanics, which is Hertzian contact mechanics that will be further discussed in the next subsection. In describing a contact deformation, the following terminology will be used: the contact radius (a), the contact penetration depth (δ) and the loading force (P) as depicted in Figure 3.5. Some major models of contact mechanics that directly incorporate surface interaction forces are summarized as follows:

DMT Mechanics [6]

This model considers long-ranged attraction and low adhesion interaction as illustrated in Figure 3.6. The tip-sample geometry remains Hertzian. The model applies to rigid systems and may underestimate the true contact area due to restricted geometry. The model is as follows:

$$P = \frac{Ka^3}{R} - 2\pi RW_{ts} \quad (3.15)$$

$$\delta = \frac{a^2}{R} \quad (3.16)$$

$$\frac{1}{R} = \frac{1}{R_{\text{tip}}} + \frac{1}{R_{\text{sample}}}$$
$$\frac{1}{K} = \frac{3}{4} \left[\left(\frac{1 - \nu_t^2}{E_t} \right) + \left(\frac{1 - \nu_s^2}{E_s} \right) \right]$$

where R is the reduced tip-sample curvature, K is the reduced tip-sample elastic modulus, ν_t and ν_s are Poisson ratio of the tip and the sample, respectively. E_t and E_s are elastic moduli of the tip and the sample, respectively. $W_{ts} = 2\sqrt{\gamma_t\gamma_s}$ is the work of adhesion of the tip and the sample, γ_t and γ_s are surface energy of the tip and the sample, respectively.

JKR Mechanics [6]

This model considers short-ranged attraction within the contact area and low adhesion interaction as illustrated in Figure 3.6. The tip-sample geometry is not necessarily Hertzian. The model applies to highly adhesive systems with low stiffness

displaying adhesion hysteresis. The model is as follows:

$$P = \frac{Ka^3}{R} - \sqrt{6\pi W_{ts}Ka^3} \quad (3.17)$$

$$\delta = \frac{a^2}{R} - \frac{2}{3}\sqrt{\frac{6\pi W_{ts}a}{K}} \quad (3.18)$$

$$\frac{1}{R} = \frac{1}{R_{\text{tip}}} + \frac{1}{R_{\text{sample}}}$$

$$\frac{1}{K} = \frac{3}{4} \left[\left(\frac{1 - \nu_t^2}{E_t} \right) + \left(\frac{1 - \nu_s^2}{E_s} \right) \right]$$

where R is the reduced tip-sample curvature, K is the reduced tip-sample elastic modulus, ν_t and ν_s are Poisson ratio of the tip and the sample, respectively. E_t and E_s are elastic moduli of the tip and the sample, respectively. $W_{ts} = 2\sqrt{\gamma_t\gamma_s}$ is the work of adhesion of the tip and the sample, γ_t and γ_s are surface energy of the tip and the sample, respectively.

Maugis Mechanics [42], [6]

This model incorporates both DMT and JKR models just by selecting the appropriate parameter λ . As λ goes to infinity, the Maugis model approaches the JKR model. On the other hand, the Maugis model resembles the DMT model as λ goes to zero. Carpick et al. discuss procedures on how to determine which model is best suited for obtained experimental data [11]. The model characterization is as follows:

$$\lambda = \frac{2.06}{\xi_o} \left(\frac{RW_{ts}^2}{\pi K^2} \right)^{1/3} \quad (3.19)$$

$$P = \frac{Ka^3}{R} - \lambda a^2 \left(\frac{\pi W_{ts} K^2}{R} \right)^{1/3} \left(\sqrt{m^2 - 1} + m^2 \arctan \sqrt{m^2 - 1} \right) \quad (3.20)$$

$$\delta = \frac{a^2}{R} - \frac{4\lambda a}{3} \left(\frac{\pi W_{ts}}{RK} \right)^{1/3} \sqrt{m^2 - 1} \quad (3.21)$$

$$1 = \frac{\lambda a a^2}{2} \left(\frac{K}{\pi R^2 W_{ts}} \right)^{2/3} \left[\sqrt{m^2 - 1} + (m^2 - 2) \arctan \sqrt{m^2 - 1} \right] \\ + \frac{4\lambda^2 a}{3} \left(\frac{K}{\pi R^2 W_{ts}} \right)^{1/3} \left[1 - m + \sqrt{m^2 - 1} \arctan \sqrt{m^2 - 1} \right] \quad (3.22)$$

$$\frac{1}{R} = \frac{1}{R_{\text{tip}}} + \frac{1}{R_{\text{sample}}} \\ \frac{1}{K} = \frac{3}{4} \left[\left(\frac{1 - \nu_t^2}{E_t} \right) + \left(\frac{1 - \nu_s^2}{E_s} \right) \right]$$

where R is the reduced tip-sample curvature, K is the reduced tip-sample elastic modulus, ν_t and ν_s are Poisson ratio of the tip and the sample, respectively. E_t and E_s are elastic moduli of the tip and the sample, respectively. $W_{ts} = 2\sqrt{\gamma_t \gamma_s}$ is the work of adhesion of the tip and the sample, γ_t and γ_s are surface energy of the tip and the sample, respectively. ξ_o is the interatomic equilibrium separation at the tip-sample interface, m is the ratio of the width of the annular region to the contact area a [64].

Figure 3.6: Stress distribution for the continuum contact mechanics model [55]

3.2.2 The Proposed Contact Model

This work considers Hertzian contact mechanics model, which is a continuum contact model that describes the contact deformation between a spherical tip and a spherical sample without any surface interactions. Unlike other models of nano contact mechanics discussed in the previous subsection, Hertzian contact mechanics do not account for surface interaction forces between two objects as illustrated in Figure 3.6. Any possible surface interactions such as adhesion and electrostatic forces are separately modeled in the interaction force module as addressed in Section 3.1.1. Figure 3.5 illustrates a simple contact deformation of a spherical tip and a spherical sample. The resulting contact radius (a) and the loading force (P) are calculated by Hertzian contact mechanics model using the necessary information of the contact penetration depth (δ) that is discussed in Section 3.1.1. The sign reversal in the penetration depth δ is needed to keep the value of δ positive to calculate for its corresponding contact radius a . The Hertzian contact model is as follows [6]:

$$a = \sqrt{R\delta} \quad (3.23)$$

$$P = \frac{4}{3} \frac{E^* a^3}{R} \quad (3.24)$$

where δ is given in eq. (3.9), E^* and R are given in eq. (3.7) and eq. (3.8), respectively.

Chapter 4

Energy Dissipation Mechanism

A perturbed system will only sustain its oscillatory motion in an ideal case where there is no energy dissipation. Otherwise, the oscillation will decay with time and eventually vanish at steady state condition. Unfortunately, some form of dissipation mechanism exists in any system in a real-life situation. In mechanical systems, the most common energy dissipation is in the form of damping. The damping mechanism may arise from internal molecular friction, sliding friction, or viscous damping due to fluid resistance [71]. The following sections will first discuss a simplified damping model and then friction from macro to atomic perspectives. Finally, nano friction models from the literature will be reviewed and compared against the proposed friction model that is used to describe the friction module of the nanomanipulation model illustrated in Figure 1.3.

4.1 Linear Damping Dissipation

Fluid damping is generally nonlinear in nature. Air resistance, for instance, is proportional to the velocity square of a moving object. The complexity of the non-

linear model is not suitable to convey the damping analysis. Nevertheless, damping can be effectively analyzed by utilizing a simple linear viscous damping model [71]. In this simplified model, the amount of damping is proportional to the velocity of the moving object in a viscous environment. The proportionality constant is referred as the viscosity constant. A higher viscosity constant will yield a higher damping on the moving object. As an illustration, an object will encounter a greater viscous resistance as it drags across an oil medium than as it drags across water as its medium. Fluids that obeys the linear damping property are known as Newtonian fluids. This section will restrict the damping analysis to Newtonian fluids.

Figure 4.1: Dissipated energy in an ideal dashpot [71]

Consider the following spring-mass-damper system with the spring stiffness k , the damping constant c , and the mass m :

$$m\ddot{x} + c\dot{x} + kx = 0 \quad (4.1)$$

The damping force F_D provides the dissipation mechanism to the system and is given by $c\dot{x}$. The dissipated energy is the closed integral of the work function:

$W_D = \oint F_D \cdot dx$. If the solution of equation (4.1) takes the form given below:

$$x(t) = X \sin(\omega t - \phi) \quad (4.2)$$

$$\dot{x}(t) = \omega X \cos(\omega t - \phi)$$

the energy loss per cycle will then be given by [71]:

$$\begin{aligned} W_D &= \oint F_D \cdot dx = \int_0^{\frac{2\pi}{\omega}} c[\omega X \cos(\omega t - \phi)]\omega X \cos(\omega t - \phi) dt \\ W_D &= \int_0^{\frac{2\pi}{\omega}} c\omega^2 X^2 \cos^2(\omega t - \phi) = (c\omega\pi X^2) dt \end{aligned} \quad (4.3)$$

The dissipated energy by the linear viscous damping can also be presented by plotting the dissipative force F_D against the displacement amount x . The shape of the plot can be determined by collecting the dissipative force and the displacement amount, and having them re-arranged as follows [71]:

$$\left(\frac{F_D}{c\omega X} \right)^2 + \left(\frac{x}{X} \right)^2 = 1 \quad (4.4)$$

According to equation (4.4), the shape of the plot is a family of an elliptical orbit. Figure 4.1 better illustrates a shape of the dissipated force as it is plotted against the displacement amount. Note that the enclosed area is the dissipated energy loss per cycle as discussed above.

4.2 Friction

Friction is an integral part to our daily lives whether it is desired or undesired. The functionality of friction is very broad but also dilemmatic in the sense that there is a sheer delineation between its adverse and favorable effects. The car industry, for instance, has run extensive research to decrease fuel consumption of its products by minimizing the undesirable friction occurring among the moving car parts. But, friction can not be entirely ruled out of the cars because of its desirable properties such as traction and braking. Instead of minimizing, a race car design has even a tendency to maximize its wheel traction and braking performance.

Long before its independent discovery by Leonardo da Vinci (1452-1519) and Guillaume Amontons (1663-1705) [23], Amonton's Law had indeed revolutionized technologies in the ancient world [7]. In the ancient world, the Egyptians were well known for constructing magnificent pyramids. The pyramids have such an immense structure that makes one wonder how the Egyptians had the parts transported and even cleverly stack-wise arranged. Egyptian scholars must have used the principle in the first Amonton's Law saying that frictional force of an object is proportionally related to normal force of the object ($f = \mu N$). They were aware that a macroscopic object is easier to slide to have it moved to another location. In sliding, friction is the only force that needs to be encountered. It also turns out that the friction of an object has mostly lower values than the object normal force ($0 < \mu < 1$). The reduction of the coefficient of friction can be further enhanced by adding a lubricant

(i.e water, oil) to the sliding surface.

In the modern world, the law has been taken for granted and is used in almost every aspect of engineering designs. Although it works for many applications, the law does not describe the complete friction phenomena. The second Amonton's Law says that friction force is independent of the contact area. This law becomes questionable when adhesion takes place during the sliding process where wear and deformation of surface structure occur. A century later, Charles Augustin Coulomb added the third law stating that friction force is independent of velocity during motion. Along with his contribution to the third friction law, Coulomb observed static and kinetic friction as well. The last friction law also only holds for macroscopic objects as it breaks down at the nano level [7].

Researchers have been struggling to resolve the above mentioned friction anomalies since the past few decades. The invention of the scanning tunneling microscope and the atomic force microscope have enabled researchers to probe friction properties down to the nano level. They found that nano friction has major differences than its macroscopic counterpart. Unlike the macroscopic friction, the interacting nano objects are super light and show sign of almost no wear as they rub against each other [7]. Nevertheless, defects on the nano structure may occur either naturally or due to high loading during the dragging process. Other important differences are that nano friction is velocity dependent [32] and exhibits stick-slip behavior that is usually irregular in terms of friction magnitude and spacing distance between the

current and the next jump [29, 4, 56]. Some researchers also show that nano friction has superlubricity characteristic that results in ultra-low energy dissipation in the friction loop as illustrated in Figure 4.2 [36, 17, 65].

Figure 4.2: Nano friction characteristics: a. typical stick slip response b. superlubricity response

Experimental data also show that nano friction is dependent on environmental condition such as temperature and humidity [37]. Consistent empirical data can be obtained only if the experiment is carried out in a controlled environment where the degree of cleanliness, the preset temperature and humidity can be maintained.

Figure 4.3: Silicon stack [46]

Nano friction has other interesting properties such as the dependency on crystallographic orientation of the surface and scanning speed [37]. The surface has a pattern

determined by the atomic compositions that make up the surface. The surface of silicon sample, for instance, will be more regular than the surface of sodium chloride sample. Schematics of both silicon and sodium chloride sample surfaces are illustrated in Figure 4.3 and Figure 4.4, respectively. As an implication of various surface patterns, a certain crystallographic orientation has an ultra-low friction dissipation and lower friction magnitude compared to other orientations [29]. In addition to the crystallographic effect, the stick slip friction magnitude keeps diminishing as the scan velocity increases [5].

Figure 4.4: Sodium Chloride stack [74]

In addition to the crystallographic orientation, substrate roughness and geometry also influence the adhesion of interacting media. The adhesion force increases if the effective contact area increases and vice versa. Substrate roughness has considerable impact on the effective contact area. The actual contact area will differ significantly from the ideal contact area due to the presence of undesired asperities that cause the ideal contact to become rough [18]. Figure 4.5 shows an example of an idealized contact between the tip and the surface of a stage at a low applied load [13].

Figure 4.5: Tip-stage idealized contact schematic [13]

4.3 Friction Modeling

Atomic friction is thus far a conundrum to scientists and researchers. Although many models such as classical and quantum friction models have been proposed for atomic friction, they have not completely described the friction phenomena. Researchers still conduct extensive research to better understand atomic friction. As a complement to the on going research on atomic friction, this work will solely focus on utilizing a classical friction model to help describe atomic friction.

Macroscopically, classical friction models are divided into two major categories, which are static and dynamic models. The Coulomb friction model is the most simplified example of the static friction model that is well known for its uses of signum function. Researchers then extend the Coulomb model with incorporating appropriate additional terms to help describe the observed dynamic phenomena during experiments such as the viscous friction, static friction (stiction), and Stribeck effect [19, 48].

Unfortunately, the mentioned static friction models have two major shortcomings. Firstly, the static models are in the form of a discontinuous function that does not have a solution (based on the existence theorem of differential equation) if the models are incorporated in the equations of motion. Secondly, static friction models rely on conditional functions to describe the presliding condition where the object being pushed has to exceed its corresponding static friction before it starts moving [19]. Disregarding their weaknesses, researchers have used static friction models to help explain atomic friction phenomena [45, 53, 68].

Considering these two major shortcomings of static friction models, dynamic friction models were developed to account for presliding condition that the static friction model lacks and to eliminate the delicate conditional functions. The dynamic friction models are mostly in the form of continuous first order differential equation [19]. Hence, the dynamic friction models are guaranteed to have at least a solution by the existence theorem. The presliding condition is also inherent on each dynamic friction model.

4.4 Dynamic Nano Friction Models in Literature

Stick slip responses are the main characteristic of nano friction. In nano friction literature, there are some dynamic nano friction models exhibiting stick slip responses. Stick slip responses of those dynamic friction models are formulated as a response of an object lying on a stage that is being pulled/pushed through a spring with a given

stiffness. The object will experience opposing force that comes from the friction between the object and the stage surface.

The modeling of the pulled/pushed object with dynamic nano friction models found in the literature are given in model 1 to model 4. Whereas the stick slip response in model 5 is defined in term of stress strain relationship. The complete description of each model is as follows:

Model 1 ([10])

$$\begin{aligned} \ddot{x} + \dot{x} &= Vt - f_1 \\ f_1 &= \begin{cases} (-\infty, \theta] & \text{for } \dot{x} = 0 \\ \theta + \beta\dot{x} & \text{for } \dot{x} > 0 \end{cases} \\ \dot{\theta} &= \frac{\theta(1 - \theta)}{\tau} - \alpha\theta\dot{x} \end{aligned} \tag{4.5}$$

where V is the desired pushing/pulling velocity, t is time. τ , α , and β are parameter constants.

The position and velocity of the object being pushed/pulled are denoted by x and $\dot{x}$, respectively. The state variable θ in model 1 represents the state of lubrication at the contact interface. The lubrication is in a full solid state (sticking phase) when $\theta = 1$. On the other hand, the lubrication is in fluid state (slipping phase) when $\theta = 0$. The model makes use of switching functions as defined in f_1 to achieve its stick slip functionality. The dissipative friction functionality is achieved in a similar way to the static coulomb friction model, but with the addition of state variable θ .

Model 2 ([48])

$$\ddot{x} + x = Vt - f_2 \quad (4.6)$$

$$f_2 = F_c + (F_s - F_c)\theta + \beta\dot{x}$$

$$\dot{\theta} = \frac{\theta(1 - \theta)}{\tau} - \alpha\theta\dot{x}$$

where F_c and F_s are dynamic and static friction values, respectively. V is the desired pushing/pulling velocity, t is time. τ , α , and β are parameter constants.

The position and velocity of the object being pushed/pulled are denoted by x and $\dot{x}$, respectively. The state variable θ in model 2 represents the state of lubrication at the contact interface. The lubrication is in a full solid state (sticking phase) when $\theta = 1$. On the other hand, the lubrication is in fluid state (slipping phase) when $\theta = 0$. Note that model 2 is an extended version of model 1 with the difference in the friction f_2 definition. The model may have made use of switching functions as implicitly discussed in the book reference [48] to achieve its stick slip functionality. The model may also use the coulomb friction approach to achieve its dissipative friction functionality.

Model 3 ([48])

$$\ddot{x} + x = Vt - f_3 \quad (4.7)$$

$$f_3 = F_c + (F_s - F_c)\theta + \beta\dot{x}$$

$$\dot{\theta} = \frac{\theta(1-\theta)}{\tau} [-\ln(1-\theta)]^{2/3} - \alpha\theta\dot{x}$$

where F_c and F_s are dynamic and static friction values, respectively. V is the desired pushing/pulling velocity, t is time. τ , α , and β are parameter constants.

The position and velocity of the object being pushed/pulled are denoted by x and $\dot{x}$, respectively. The state variable θ in model 3 represents the state of lubrication at the contact interface. The lubrication is in a full solid state (sticking phase) when $\theta = 1$. On the other hand, the lubrication is in fluid state (slipping phase) when $\theta = 0$. Note that model 3 is also an extended version of model 1 with the difference in the new definition of rate of state variable $\dot{\theta}$.

Model 4 ([48])

$$\ddot{x} + x = Vt - f_4 \quad (4.8)$$

$$f_4 = F_c + (F_s - F_c)(1 - e^{-(\theta/\tau)}) + \beta\dot{x}$$

$$\dot{\theta} = 1 - \theta\dot{x}/D$$

where F_c and F_s are dynamic and static friction values, respectively. V is the desired pushing/pulling velocity, t is time. D , τ , and β are parameter constants.

The position and velocity of the object being pushed/pulled are denoted by x and $\dot{x}$, respectively. The state variable θ in model 4 corresponds to the bristle deflection of the object with respect to contact surface similar to the state in *LuGre* friction model. In the pushing/pulling direction, the lower bound of θ is zero that corresponds to no deflection case. The upper bound of θ is $D/\dot{x}$ representing the bristle maximum deflection before the bristle slips into the next sticking phase, respectively. The model may have made use of switching functions as implicitly discussed in pp. 360 and Figure 12.8 in the book reference ([48]) to achieve its stick slip functionality. The model may also use the coulomb friction approach to achieve its dissipative friction functionality.

Model 5 ([39, 40])

$$\begin{aligned}\ddot{x} &= -E_1 e^{-\kappa/\dot{x}} + \alpha \sigma \dot{\gamma} \\ \dot{\sigma} &= \mu(\dot{\epsilon} - \dot{\gamma}) \\ \dot{\epsilon} &= V/2h \\ \dot{\gamma} &= E_0 e^{-1/\dot{x}} \sinh\left(\frac{\sigma}{\bar{\mu}}\right)\end{aligned}\tag{4.9}$$

where V is the desired pushing/pulling velocity, E_0 , E_1 , κ , μ , h , α , and $\bar{\mu}$ are parameter constants.

The position and velocity of the object being pushed/pulled are represented by x and $\dot{x}$, respectively. The term $\dot{\epsilon}$ and $\dot{\gamma}$ denote the rate of elastic shear deformation

and the rate of plastic shear deformation, respectively. The positive net rate of shear deformation ($\dot{\epsilon} - \dot{\gamma}$) corresponds to forward slipping phase. Whereas the sticking phase occurs when the net rate of shear deformation is zero. $\dot{\sigma}$ represents the rate of shear force due to the net rate of shear deformation. In this particular model, the forcing input Vt found in other models are embedded in the $\dot{\sigma}$ rate equations as the constant rate of elastic shear deformation $\dot{\epsilon}$. The model does not rely on any switching function to achieve its stick slip and dissipative property.

4.4.1 Analysis of The Dynamic Nano Friction Models

This section presents the analysis of the dynamic nano friction models found in the literature via numerical simulations. The numerical simulations were carried out to determine the effectiveness of the models in exhibiting energy dissipation and stick slip friction responses.

Responses of Model 1

Paper version: The object will experience sticking ($\dot{x} = 0$) and slipping phase ($\dot{x} > 0$) in an alternating pattern as illustrated in the bottom left plot of Figure 4.6. During the sticking phase, the state variable θ starting from a nonzero initial value increases to its maximum value ($\theta_{max} = 1$) and stay there. The friction force is assumed to be equal and opposite to the applied force during the sticking phase just like the situation in static coulomb friction model. The state variable θ will drop to its minimum value other than zero when the object slides. The spring force is defined

as $F_{spr} = -(x - Vt)$ and behaves accordingly as illustrated in the top left plot of Figure 4.6.

Figure 4.6: Model 1 stick slip responses taken from [10]

MATLAB verification: The simulation results for model 1 cannot be reproduced by simply solving the given equations with the given parameters. The simulation results of model 1 are successfully reproduced by implementing the do not push/push scheme that conforms to the definition of f_1 as shown in Figure 4.7.

Figure 4.7: Model 1 stick slip simulation responses via a switching scheme

Without Coulomb - like switching function, these dynamic friction models act as an active input source to the system. Suppose that all of the system in model 1 starts from equilibrium condition. When there is no external forcing term (Vt), the systems will instead keep moving in the reverse direction for all nonzero θ_0 initial condition. The system will stay in equilibrium if θ_0 is zero.

Figure 4.8: Model 1 stick slip simulation responses (Limit Cycle case)

Book version: Model 2 does not display sticking phase. Instead, the object creeps in the reverse direction before it slides forward during the slipping phase as observed in position x plots in Figure 4.9. During the creeping phase, the state variable θ starting from a nonzero initial value increases to its maximum value ($\theta_{max} = 1$) and stay there. The state variable θ will drop to its minimum value other than zero when the object slides. The spring force is defined as $F_{spr} = -(x - Vt)$ and exhibits softening effect as illustrated in Figure 4.9 during its creep-slip responses.

Figure 4.9: Model 2 creep slip responses taken from [48]

MATLAB verification: The simulation results for model 2 cannot be reproduced by simply solving the given equations with the given parameters. Appropriate switching functions must have been used to obtain the simulation results. The following discussions apply to the case where the model does not use any switching functions. Figure 4.8 illustrates the numerical solution to model 1 when the model parameter

β is further tuned down to get to the limit cycle. Observe that the resulting spring response of Figure 4.8 looks like the pattern of the state variable θ in right plot of Figure 4.9. Other responses of model 2 as shown in Figure 4.9 are still not reproducible. In MATLAB simulation, the direct solution to model 3 stalls at the time when the friction state variable θ goes to one. The undesired active friction behavior also applies to model 2 and 3 if Coulomb - like switching friction scheme is not implemented.

Figure 4.10: Model 4 stick slip responses taken from [48]

Responses of Model 4

Book version: Figure 4.10 shows spring force $F_{spr} = -(x - Vt)$ responses of model 4 when spring stiffness is gradually varied from the lowest to the highest value. The

pushing/pulling velocity is also varied from the lowest to the highest value for each stiffness case.

For low stiffness case, the stick-slip response of the spring force diminished in an overdamped fashion (the convergence of the spring force converges to its corresponding kinetic value) as the velocity is increased. On the other hand, the stick-slip response of the spring force diminished in an underdamped fashion (the convergence of the spring force converges to a value between its corresponding kinetic and static values) as the velocity is increased. Other model responses such as the object velocity and the profile of the state variable were not made available in the book.

Figure 4.11: Model 4 stick slip simulation responses (parameters in case b)

MATLAB verification: Without implementing appropriate switching functions, none of the plots in Figure 4.10 is reproducible in MATLAB as shown in Figure 4.11 for case b when the spring constant is 360 [N/m]. In steady state, the spring force

instead varies linearly with time in a decreasing fashion as shown in the bottom right plot of Figure 4.11. The position x of the object will vary linearly with time in an increasing fashion due to the ramped external pushing/pulling force as the position plot of Figure 4.11 zoomed in MATLAB. When the parameter β is further tuned to a sufficiently low value, the system response will go into a limit cycle that preserves the oscillatory motion of both the object position x and the object velocity $\dot{x}$. Without Coulomb - like switching function, the friction model in model 4 also acts as an active input source to the system. Suppose that all of the system in model 1 starts from equilibrium condition. Without external forcing term (Vt), the systems will instead move and converge to a position in the reverse direction for any initial conditions.

Responses of Model 5

Paper version: The steady state responses of the model that are illustrated in Figure 4.12 are as follows. The shear force will first go to its maximum value while the object slips at a low rate. As the object is kept pushed, the shear force drops to its minimum value while slip rate increases. The velocity of the object is bounded as the energy is dissipated by the built-in friction term $E_1 e^{-\kappa/\dot{x}}$. The cycle then repeats.

MATLAB verification: Unlike the other dynamic friction models, the creep-slip responses of model 5 are reproducible by directly solving the given differential equations with the given parameters as shown in Figure 4.13. The undesired creeping motion during the stiction phase of the stick slip friction responses is the major deficiency of the friction model as presented in the papers. The creep motion is expected because the system in model 5 will stay in equilibrium if the velocity $\dot{x}$ is zero.

Figure 4.12: Model 5 stick slip responses taken from [40]

The creeping motion of model 5 can be observed in the plot of mass position during sticking phase in Figure 4.13. Another explanation of the creeping motion may come from the built-in friction term $E_1 e^{-\kappa/\dot{x}}$. For the unforced system with a nonzero initial velocity $\dot{x}(0)$, the sliding mass will only stop as time goes to infinity. In addition to the undesired creeping motion, model 5 has more state variables than *LuGre* friction model although some states such as ϵ and γ can be eliminated because they do not directly contribute the overall system.

Figure 4.13: Model 5 stick slip simulation responses

4.4.2 Discussion of The Dynamic Nano Friction Models

In summary, five nano dynamic friction models were found in literature. Model 1 introduces a state variable as a measure of the lubrication state at the contact interface. Models 2 and 3 are extensions of model 1. Model 4 has a state variable corresponding to the bristle deflection of the object with respect to contact surface similar to the state in *LuGre* friction model. Model 5 is derived from the shear transformation zone (STZ) theory that defines its states as shearing stress, plastic and elastic strain.

These nano dynamic friction models have certain disadvantages in exhibiting the stick slip responses. Models 1 to 4 rely on Coulomb-like switching function to achieve the energy dissipation property and implement certain conditional switching functions to obtain the stick-slip friction responses. The utilization of such switching functions undermine the goal of this work, which is to account for the presliding and transient

responses. Although model 5 reproduces stick-slip friction responses without switching functions, it suffers from the undesired creeping motion during the sticking phase. Such undesired creeping motion is also observed in models 2 and 3. In addition to the undesired creeping motion, one of the states in model 5, the free volume that can be correlated as a sliding mass velocity, needs infinite time to come to a complete stop for a nonzero initial condition.

4.5 Extended *LuGre* Dynamic Friction Model

Unlike dynamic nano friction models found in the literature, *LuGre* friction model is truly a well posed dynamical model that reliably acts as energy dissipation mechanism, accounts for presliding phase, and exhibits stick - slip response. *LuGre* friction model has been rigorously analyzed and possesses mathematical properties such as existence and uniqueness of solution, boundedness of solution, and dissipativity [47, 19].

Figure 4.14: LuGre friction model [47]

The friction model uses the bristle deflection as its state. The bristle can be thought of as a cantilever rigidly connected to a body that deflects and slips through

a terrain as the body is dragged across a surface. Figure 4.14 better illustrates the schematic of the *LuGre* friction model. In addition to having the mentioned mathematical properties, *LuGre* friction model also facilitates appropriate parameter tuning to obtain friction response as shown in Figure 4.15. Olsson [47] discusses extensively preliminary ways to tune the parameters to get a desired friction response. Therefore the *LuGre* friction model with proper parameter tuning will be used in this work to characterize the nano friction interaction between the sample and the stage as follows:

$$F_{\text{rict}} = \sigma_0 b_s(t) + \sigma_1(\dot{y}_s(t)) \frac{db_s(t)}{dt} + F_v \dot{y}_s(t) \quad (4.10)$$

$$\frac{db_s}{dt} = \dot{y}_s - \frac{|\dot{y}_s|}{g(\dot{y}_s)} b_s \quad (4.11)$$

$$g(\dot{y}_s) = \frac{1}{\sigma_0} \left[F_c + (F_s - F_c) e^{-(\dot{y}_s/v_s)^2} \right]$$

$$\sigma_1(\dot{y}_s) = \sigma_1 e^{-(\dot{y}_s/v_d)^2}$$

where $b_s(t)$ is bristle deflection, $\dot{y}_s(t)$ is the sample velocity along the pushing axis, F_s and F_c are the static and kinetic friction magnitudes, respectively, σ_0 is bristle stiffness, σ_1 is bristle damping coefficient, F_v is the viscous damping coefficient, v_s is Stribeck velocity constant, and v_d is a velocity constant.

Besides stick slip responses, the dependency on sliding velocity is another characteristic of nano friction. Experimental data show that both static and kinetic friction magnitudes converge to a friction value between the static and the kinetic friction in a certain way as the sliding velocity increases [37, 5]. Zwörner et al. [76] and Meurk

Figure 4.15: LuGre friction model response [47]

[45] experimentally show that frictional forces are independent of the sliding velocity in a wide interval of sliding velocity. Other experimental data show that the mean lateral friction increases in a certain way as the sliding velocity increases [48, 46]. Modified Tomlinson friction model is a particular example that describes the friction dependency on the sliding velocity. According to the model, the mean friction force logarithmically increases with increasing velocity v as given below [46, 32]:

$$F_m(v, T) = F_{m,0} + \frac{k_B T}{\lambda} \ln \left(\frac{v/a}{f_0} \frac{\lambda k_{\text{eff}} a}{k_B T} \right) \quad (4.12)$$

where F_m is the mean lateral friction force, $F_{m,0}$ is the initial mean lateral friction force, a is the lattice constant of the surface in the scan direction, v is the sliding velocity, T is the surrounding temperature, k_B is the Boltzman's constant, k_{eff} is the effective lateral spring constants, $\lambda = \frac{k_B T}{F_{m,1}}$ is a length parameter related to the distance involved in the slip, $F_{m,1}$ is the mean absolute value of the peaks in the friction loops, and f_0 is the characteristic frequency.

The original *LuGre* friction model has an inherent sliding velocity dependency property. But, the velocity dependency is only significantly observable in more than 2 order magnitude of velocity differences. This work extends the *LuGre* friction model to enhance the sliding velocity dependency of nano friction so that the property is directly tunable as desired. Thereby, the following modifications of the static friction F_s and kinetic friction F_c are proposed to the original *LuGre* friction model:

$$\begin{aligned} F_s(\dot{y}_b) &= F_{s,\min} + (F_{s,\max} - F_{s,\min})e^{-\frac{1}{C}(\dot{y}_b - v_{\min})}, \quad \dot{y}_b \geq v_{\min} \\ F_c(\dot{y}_b) &= F_{c,\max} + (F_{c,\min} - F_{c,\max})e^{-\frac{1}{\alpha C}(\dot{y}_b - v_{\min})}, \quad \dot{y}_b \geq v_{\min} \end{aligned} \quad (4.13)$$

where $\dot{y}_b$ is the given tip base pushing velocity, $v_{\min}$ is arbitrary minimum velocity, α and C are constants.

The resulting extended *LuGre* friction model has a total of twelve parameters to tune in comparison to a total of seven parameters in the original model. The major modification of the original *LuGre* friction model is only to the static and kinetic friction, which are now a function of the tip base pushing velocity $\dot{y}_b$. The modified friction model still inherits the mathematical properties of the original model because the newly defined static and kinetic frictions are bounded functions. Note that similar approaches to the enhancement of the velocity dependency can also be generalized to account for other environmental dependencies such as humidity, temperature, etc.

In the extended *LuGre* friction model, the static and kinetic frictions are assumed to vary exponentially with respect to the pushing velocity as they converge to their

Figure 4.16: Static and dynamic friction dependency on the tip base pushing velocity respective convergent values, i.e. $F_{c,\max}$ and $F_{s,\min}$. In fact, Scherge et al. [55] present experimental data that show a good agreement with exponential curve fit for the stick -slip amplitude convergence as a function of sliding velocity. The percentage amount of each convergence starts at a corresponding critical pushing velocity $\dot{y}_{b,\text{crit}}$. The static and kinetic dependency on pushing velocity is better illustrated in Figure 4.16. Note that the convergent values, $F_{c,\max}$ and $F_{s,\min}$, can be equal to each other according to the above mentioned experimental data [5].

Chapter 5

Simulations

This chapter will discuss some model responses that are dependent on both initial conditions and parameters. A simulation scenario will be first introduced to show the non-contacting initial conditions of the system. The forced system responses with some sets of parameters will then be presented to demonstrate the system dependency on parameters. The forced system will be tuned in such a way as to exhibit interesting nano friction characteristics such as the stick slip motion, velocity dependency, superlubricity, and jump to contact phenomenon. Finally, all of the simulation results will be briefly summarized and discussed in Section 5.3.

5.1 Model Responses for the Initial Set of Parameters

This section shows via simulations that the proposed nanomanipulation model behaves as discussed in Chapter 1. The introduction of *LuGre* friction model helps exhibit the stick slip friction response. The tip - sample interaction model improves contact modeling to fully account for transient responses of the nanomanipulation. Simulations in the next few sections assume boundary lubrication that contributes to

viscous damping being negligible in the friction subsystem. For the sake of clarity, the resulting nanomanipulation model is summarized as follows:

$$m_t \ddot{y}_t(t) + c_t \dot{y}_t(t) + k_t y_t(t) = c_t \dot{y}_b + k_t y_b(t) - F_{ts}(\tilde{y}(t))$$

$$m_s \ddot{y}_s(t) = F_{ts} - F_{\text{rict}}$$

$$\frac{db_s}{dt} = \dot{y}_s - \frac{|\dot{y}_s|}{g(\dot{y}_s)} b_s$$

$$F_{ts}(\tilde{y}(t)) = \text{Interaction Force}$$

$$F_{\text{rict}} = \text{Friction}$$

The summarized equations are a 5 - state dynamics model. After transforming the proposed model into its corresponding state space formulation, the resulting state space representation is then implemented in MATLAB, a numerical simulator. Coupled modules that are illustrated in Figure 1.3 constitute the following equations: eq. (2.11), eq. (2.13), eq. (3.6), and eq. (4.10). These coupled equations are simultaneously solved via a stiff MATLAB ODE solver, which is the ODE 23 TB, with appropriate error tolerances. The resulting penetration depth $\delta(t)$ is then used to determine corresponding contact radius $a(t)$ and loading $P(t)$ via Hertzian Contact Mechanics analysis described in eq. (3.23) and eq. (3.24), respectively.

The remainder of this section will be organized as follows. The initial nanomanipulation setup along with selection of model parameters will be given in Section 5.1.1. Section 5.1.2 will present the initial jump to contact phenomenon observed in the simulation results. The stick slip model responses will then be presented in Section 5.1.3. The corresponding contact properties of the simulation results will be analyzed in Section 5.1.4.

Table 5.1: Simulation parameters for the jump to contact case

Parameter	Value	Unit
F_s	1×10^{-9}	N
F_c	6×10^{-10}	N
σ_0	1×10^5	N/m
σ_1	1.5×10^{-6}	N.s/m
v_s	1×10^{-5}	m/s
v_d	0.1	m/s
F_v	0	N.s/m
ρ_{tip}	2330	kg/m ³
ρ_{sample}	2330	kg/m ³
m_t	1.98×10^{-18}	kg
m_s	4×10^{-17}	kg
c_t	7.01×10^{-9}	N.s/m
k_t	26.67	N/m
R_{tip}	50×10^{-9}	m
R_{sample}	160×10^{-9}	m
a_o	3.75×10^{-10}	m
ν_t	0.33	none
ν_s	0.33	none
E_t	210	GPa
E_s	0.77	GPa
H	1.452×10^{-20}	J
Solver	ODE 23 TB	none
RelTol	10^{-5}	none
AbsTol	10^{-15}	none

5.1.1 Simulation Scenario

A simple schematic of possible nanomanipulation setups is illustrated in Figure 5.1. The initial conditions are designed in such a way as to start a simulation with the tip and the sample not being in contact. The selection of non-contacting initial conditions is to demonstrate the extended coverage of the proposed model to include both contacting and non-contacting initial conditions. On this occasion, parameters of the proposed model are tuned to the set of parameters tabulated in Table 5.1.

Figure 5.1: Possible setup of the AFM pushing manipulation: a. non-contacting case and b. contacting case

The detail of the nanomanipulation setup is as follows. In the simulation, the sample diameter is assumed to be larger than the tip diameter. The nanomanipulation is carried out in a vacuum environment with a proper electrical grounding. The attractive van der Waals force is expected to be the only interaction that may arise from such an environment. As the first preparation step for the manipulation, a nanosphere is deposited on the stage. The tip is then aligned in a distance away from the sample along the pushing axis. Since the tip diameter is smaller than the sample diameter, there will be a gap between the tip and the stage that is also assumed to be maintained constant through the implementation of a feedback control. The sudden

presence of the tip induces attractive force between the tip and the sample that will be reflected in arbitrarily choosing an initial position difference $\tilde{y}$ at 4×10^{-10} m. Other initial conditions such as the tip position y_e , the tip velocity $\dot{y}_e$, the sample velocity $\dot{y}_{s,e}$, and the bristle deflection $b_{s,e}$ are assumed to be zero to match with the initial setup. The manipulation starts as soon as the tip is aligned at the desired position. The tip base is to follow a ramped position input (open loop) with a constant velocity y_b of $3 \mu\text{m/s}$ as it pushes the sample across the stage.

5.1.2 Initial Jump to Contact Phenomenon

This section will study transient forced responses of the proposed model in the first few nanoseconds. The tip has not yet done much pushing on the sample within this time frame. The model responses are largely influenced by the tip - sample interaction force. The specific case to observe is the initial jump to contact phenomenon that is illustrated in Figure 5.2. Note that any referral on jumping phenomena in the simulation results occurs continuously in time (not in an abrupt way). Selected model outputs such as the friction, the tip - sample interaction force, the tip - sample position difference $\tilde{y}$, the tip and the sample positions are presented in Figure 5.3.

Figure 5.2: A very fast transition (α is small) from a given initial non contact condition to a contact condition

According to Figure 5.3.a, the tip initially jumps forward before it bounces back somewhere in the forward pushing direction. On the other hand, Figure 5.3.b shows that the sample gradually goes in a reverse direction approaching the tip and eventually settles somewhere in the reverse pushing direction. Both tip and sample position responses can be better understood by looking at the plot of the negative position difference, i.e. $-\tilde{y}(t)$, as shown in Figure 5.3.d. Given the initial position difference of -4×10^{-10} m, the tip and the sample approach each other due to the attractive van der Waals force. The tip initially approaches faster than the sample until the tip bounces back as a result of colliding with the sample. The tip and the sample get stuck to each other with some contact deformation for some time after the collision. The resulting contact deformation will be better presented later in subsequent plots.

Next, the resulting friction and tip - sample interaction force as shown in Figure 5.3.c will be discussed. In the beginning of the pushing operation, the friction jumps to a negative value trying to resist the sample motion that is being attracted toward the tip by the attractive van der Waals force. But, the sample moves toward the tip as soon as the attractive force between the tip and the sample exceeds the breakaway force between the sample and the stage. The breakaway force is defined as the necessary amount of external force that is time rate dependent to cause a steady motion of an object encountering friction on its interface along a pushing direction [47]. Note that the resulting breakaway force is the kinetic friction magnitude F_c .

Figure 5.3: Model responses that display an initial jump to contact in the beginning of the nanomanipulation

Both friction and the tip - sample interaction force eventually equilibrate after the tip and the sample get stuck and deformed at the contact point.

5.1.3 Stick Slip Responses

Steady state forced responses of the proposed model in the first hundreds of microseconds will be studied in this section. The proposed model is expected to display a stick slip friction characteristic in its steady state responses.

Figure 5.4: Model responses that exhibit steady state stick slip responses

Selected model outputs such as the friction, the tip - sample interaction force, the contact penetration depth δ , the tip and the sample positions are presented in Figure 5.4. Figure 5.4.a and 5.4.b illustrate the behavior of the tip and the sample positions, respectively, as the tip is axially dragged across the stage. The tip position varies linearly with time and periodically experiences a jump to a higher tip position. On the other hand, the sample position always jumps periodically to a higher sample position rendering a steady stick slip motion. Note that the stick slip sample motion starts from a position lower than the given initial condition of the sample position

because of the initial jump to contact phenomenon discussed in Section 5.1.2.

The observation of the friction response and the tip - sample interaction force as shown in Figure 5.4.c will now be discussed. Since the tip - sample interaction force qualitatively follows the friction response, the discussion will simply focus on the friction response. Close to the beginning of the pushing operation, the friction jumps from a lower value to a higher value. In the sticking phase, the friction value keeps increasing with a hardening contact stiffness, which is given by the slope of the friction with respect to the tip position, until it reaches its breakaway force that corresponds to static friction value F_s for this case. The friction then slips to a fraction of the given dynamic friction F_c during the slipping phase. The steady state friction response periodically repeats rendering a stick slip pattern. Note that the friction value is initially negative indicating that the friction is resisting the sample being pulled toward the tip as previously discussed in Section 5.1.2.

The contact penetration depth $\delta(t)$ between the tip and the sample against the tip position is presented in Figure 5.4.d. The contact deformation occurs when the position difference of the tip and the sample is negative with respect to the inter-atomic equilibrium separation distance a_o as discussed in Section 3.1.1. The resulting contact penetration depth $\delta(t)$ is similar to its corresponding friction response. Note that the position difference also jumps from a non-contacting value to a contacting value close to the beginning of the pushing operation. Once the tip is in contact with the sample, the tip remains in contact with the sample in a stick slip pattern.

5.1.4 Contact Analysis

In this section, Hertzian contact mechanics model as described in Section 3.2.2 will be applied to analyze the resulting contact penetration depth $\delta(t)$. Plots of the contact radius and the contact loading against time are presented in Figure 5.5.

The profile of contact deformation during the simulated manipulation process can be better inferred from these plots. Figure 5.5.a shows the contact radius profile indicating an initial jump to contact phenomenon. According to the plot, both the tip and the sample remain in contact once they come in contact. In the sticking phase, the profile of the contact area tracks a stick slip pattern with a decreasing slope steepness with respect to time. The corresponding contact loading is given in Figure 5.5.b. The profile of the contact loading also follows a stick slip pattern, but with an increasing slope steepness with respect to time in the sticking phase.

Figure 5.5: Corresponding contact radius and loading profiles of the jump to contact case analyzed by Hertzian contact mechanics

5.2 Model Responses for Other Sets of Parameters

This section will present other forced responses of the proposed nanomanipulation model that capture physical phenomena commonly observed in nano friction. The first phenomenon to be shown is the dependency of the model on an applied normal load [28, 12, 14, 13, 26]. The initial set of parameters will be adjusted in such a way as to illustrate the loading dependency. Particular emphasis is placed on tuning the magnitude of the kinetic friction F_c that directly varies with the external load such as the interaction force between the sample and the stage. The resulting adjusted parameters are tabulated in Table 5.2.

Table 5.2: Simulation parameters for superlubricity case

Parameter	Value	Unit
F_c	2.5×10^{-10}	N
v_s	1×10^{-4}	m/s
σ_1	2×10^{-6}	N.s/m
H	7×10^{-21}	J
E_s	0.51	GPa

The model responses are superimposed with responses of the jump to contact case as in Figure 5.6 (dashed lines). The pattern of the tip and the sample positions are generally similar to the ones in the jump to contact case, except that the periodicity interval increases. The increase of the periodicity interval results in the increase of the jumping magnitude of the sample position to about 0.45 nm.

Figure 5.6: Model responses that display jump to contact and superlubricity characteristics

Figure 5.6.c shows the friction response that oscillates back and forth from the positive to negative region yielding much lower dissipated energy per cycle than the friction in the jump to contact case. This low energy dissipation phenomenon is known as superlubricity [17].

The corresponding contact stiffness that is given by the slope of the friction with respect to the tip position also experiences softening effect compared to the contact stiffness in the jump to contact case. The jumping phenomenon in the jump to contact

case disappears as well. The deformation profile of the current model is illustrated in Figure 5.6.d. The resulting maximum amount of the deformation is larger than the one in the jump to contact case. Unlike the response in the jump to contact case, the tip intermittently loses contact with the sample. The jumping phenomenon in the previous deformation profile also disappears.

Table 5.3: Simulation parameters for velocity dependency case

Parameter	Value	Unit
$F_{s,\max}$	1×10^{-9}	N
$F_{s,\min}$	7×10^{-10}	N
$F_{c,\max}$	7×10^{-10}	N
$F_{c,\min}$	6×10^{-10}	N
$v_{\min}$	5×10^{-7}	m/s
C	1×10^6	m/s
α	10	none

Next, the simulation implements the extended *LuGre* friction model with the proposed modifications as in eq. (4.13) to demonstrate the dependency of the model responses with respect to a varied pushing velocity. The model mostly still uses parameters in the jump to contact case with adjusted parameters as shown in Table 5.3. Note that additional parameters are tuned in such a way as to reflect the desired friction response as shown in Figure 4.16.

The friction and the deformation responses of the model for two different pushing velocities are illustrated in Figure 5.7. The model has the following different responses as the pushing velocity is increased to ten times higher. First, the jumping phenomena on both the friction and the deformation profiles vanish. While the magnitude of the

Figure 5.7: Model responses that show the dependency on varied pushing velocities static friction decreases, the dynamic friction increases. Thereby, the mean friction increases as desired. Finally, the frequency of the stick slip oscillation increases as the pushing velocity increases. Note that the contact stiffness remains the same indicating no dependency on the pushing velocity.

Finally, Hertzian contact mechanics will be applied to analyze the contact properties of the model responses of the jump to contact case and the superlubricity case. The contact radius and the contact loading against the tip position for both cases are superimposed and presented in Figure 5.8. The deformation of the contact point can be better inferred from these plots. Figure 5.8.a shows the contact radius profile of both the jump to contact and superlubricity cases. In the jump to contact case, the contact deformation remains and tracks a stick slip pattern once the tip and the sample come in contact. On the other hand, the contact deformation follows an elliptic pattern with intermittent contact lost for the superlubricity case. The resulting maximum contact radius of the superlubricity case is also greater than the maximum

contact radius of the jump to contact case. The corresponding loading profiles of both cases are given in Figure 5.8.b. In contrast to its contact radius, the contact loading

Figure 5.8: Hertzian contact radius and loading plotted against the tip position for the jump to contact and superlubricity characteristics

of the superlubricity case is less than the contact loading of the jump to contact case. The suppression of the contact loading may be because of the ability of the sample with a lower modulus of elasticity to spread out the resulting contact pressure by having more contact area as a result of the corresponding contact deformation.

The contact radius and the contact area are further plotted against contact loading for both cases as shown in Figure 5.9 to give a different perspective of how the deformation occurs at the tip and sample contact point during the nanomanipulation. In the superlubricity case, the contact radius and the contact area responses first increase in their respective way to a maximum value, decrease to zero and lose contact for some times as can be seen in the left plots of Figure 5.9. The pattern then repeats indefinitely. Similar pattern occurs in the jump to contact case, except for differences

Figure 5.9: Comparison of contact radius and contact loading between the jump to contact and superlubricity characteristics

in the second and the last stage of the cycle indicating always in contact condition. Instead, the contact radius and the contact area first increase to a maximum value, decrease to a minimum value other than zero, and repeats the cycle as illustrated in the right plots of Figure 5.9.

5.3 Summary of Simulation Results

The simulation results that are presented in this chapter will be summarized as follows. Simulation results also show that the proposed model extends the coverage of initial conditions to include both contacting and non-contacting conditions. The tip and the sample may experience an initial jump to contact phenomenon for non-contacting initial conditions as observed in the simulation results. The proposed model exhibits a stick-slip friction response that is accompanied by the stick-slip motion experienced by the sample. The proposed model also facilitates the extraction

of a continuous contact deformation profile of the tip and the sample to further analyze contact properties such as contact loading and radius. Using other sets of parameters, the proposed model displays characteristics of nano friction such as superlubricity and enhanced velocity dependency.

Comparing the simulation results to nanomanipulation experimental data [34, 3, 24, 22, 63, 62], the results are qualitatively similar. Differences in stick-slip cycle frequency and magnitude are attributed to parametric differences. Nevertheless, simulation results show that relevant parameters (e.g. the kinetic friction F_c , the sample and the nanotip stiffness) can be further tuned to adjust the stick-slip cycle frequency and magnitude. Due to the good qualitative agreement, the prospects for tuning parameters of the proposed model to experimental data are encouraging.

Chapter 6

Conclusions

A complete nanomanipulation dynamical model that is composed of integrated modules is presented. The proposed model describes the nanomanipulation of a spherical nano object via a nanotip. The major contribution of the work comes from the introduction of *LuGre* (Lund-Grenoble) dynamic friction model [47] that helps characterize the stick-slip friction response observed in experimental data and improve the performance of static friction models. With appropriate parameter tuning, the proposed model is capable of reproducing other possible behaviors of the nanomanipulation process such as the jump to contact phenomenon of the cantilever due to the stiffness softening effect, velocity dependency, and superlubricity.

Another contribution of the proposed model is the elimination of the restrictive contacting initial conditions in existing nanomanipulation models found in the literature that require the nanotip and the sample being initially in contact before the nanomanipulation starts. The non - contacting initial conditions can now be accounted for in the proposed model. The proposed nanomanipulation model is also able to describe the entire collision process between the tip and the sample that en-

ables the extraction of continuous contact deformation profiles. The description of the complete collision process is made possible by utilizing an appropriate interaction force model as a coupling mechanism between the tip and the sample. In addition to being compliant to either physical or virtual parameter changes, the model is also more practical and efficient in computational time than the molecular dynamics model.

The proposed model can also be tailored to take other physical phenomena into consideration by improving each of its subsystems. As an example, the tip-sample interaction can be extended to accommodate adhesion, electrostatic, and magnetic interactions. The friction subsystem can be enhanced as well to consider other environmental dependencies such as humidity, temperature, and boundary lubrication. The description of physical parameter dependencies can be further refined by either direct derivations from fundamental laws of physics or curved-fitted functions of experimental data.

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