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I am submitting herewith a thesis written by Lee Peter Doane entitled “Nano-Mechanics of a Micro Cantilever Beam Excited by Interactive Atomic Forces’.” I have examined the final paper copy of this thesis for form and content and recommend that it be accepted in partial fulfillment of the requirements for the degree of Master of Science, with a major in Mechanical Engineering.


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“Nano-Mechanics of a Micro Cantilever Beam Excited by Interactive Atomic Forces”

**A Thesis Presented
for the
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at
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Abstract

The objective of this research was to predict the dynamic behavior of a micro-cantilever tip, commonly used in atomic force microscopes. This was done by examining the horizontal force component of the forces between one atom on the tip of a micro-cantilever and a single row of atoms lying within an adjacent surface. This model does not include an energy dissipation mechanism between the moving atom on the tip and the surface atoms. The system is conservative and therefore the interactive forces cannot be considered as true friction.

The atomic force microscope (AFM) is typically used to measure friction at the atomic and nano-scales, this device will be the basis for our study. In order to understand the mechanisms of friction, it is necessary to understand the dynamics of the micro-cantilever tip as it engages a surface. Therefore the focus of this analytical research, which was based on Newtonian mechanics, was to predict: 1) tip dynamics 2) related horizontal driving force. The problem is especially challenging because the analysis includes atomic forces, which leads to solving non-linear differential equations. The Newmark Beta method was used to solve the non-linear equations of motion. The horizontal driving force was obtained from the calculated motion of the micro-cantilever tip.

Three modes of vibration were examined. These were the horizontal mode and vertical mode, and then the two-dimensional mode. The two-dimensional mode allowed the tip to move in a horizontal and vertical direction independently and thus required a two degrees of freedom analysis.

The horizontal mode was driven by the surface being scanned under the micro-cantilever tip. The vibration and horizontal force in the horizontal mode had a periodic pattern to it. The horizontal force was out of phase with the vibration by ninety degrees. The vertical mode was a free vibration with the tip positioned directly over a single atom. The tip was released from different positions. This set of calculations was most useful in

checking the validity of the computer algorithm since the total energy in the conservative system was constant.

The two-degree of freedom case best simulates the actual motion of the micro-cantilever tips. For the set of input parameters used in this study, the vertical component of the tip motion was much greater than, the horizontal component. This dynamic behavior was reflected in the atomic horizontal driving force that was applied to the tip.

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List of Abbreviations and Symbols

Abbreviations

m.....	Meter
mm.....	Millimeter
cm	Centimeter
in.....	Inch
μm	Micrometer
nm.....	Nanometer
$\text{\AA}$	Angstrom
nN.....	Nano Newton
nN nm	Energy
s	Second
Hz	Hertz (1 cycle/s)
ms	Milliseconds
mV.....	Milli-Volts
J	Joule
eV	Electron Volt
K.....	Kelvin

Symbols

V_s	Scanning Velocity
ϕ	Potential Energy
R	Separation Distance between Atoms
A	Constant for the Attractive Component of the Lennard-Jones Potential, which is based on Material Properties.
B	Constant for the Repulsive Component of the Lennard-Jones Potential, which is based on Material Properties.
u.....	Horizontal Displacement of Micro-Cantilever Tip
v.....	Vertical Displacement of Micro-Cantilever Tip
k_h	Equivalent Horizontal Stiffness of Micro-Cantilever Beam
k_v	Equivalent Vertical Stiffness of Micro-Cantilever Beam
X_o	Horizontal Displacement between Surface Atoms and the Atom on the Tip of the Micro-Cantilever
Y_o	Vertical Displacement between Surface Atoms and the Atom on the Tip of the Micro-Cantilever (Also called Micro-Cantilever Vertical Offset).
AS.....	Atomic Spacing (Distance between the Centers' of two Atoms)
t.....	Time (Seconds)
F_h	Horizontal Force
F_v	Vertical Force

m	Equivalent Mass of Micro-Cantilever
f_h	Horizontal Natural Frequency of Micro-Cantilever
f_v	Vertical Natural Frequency of Micro-Cantilever
v_o	Initial Vertical Displacement of Tip for Vertical Mode Vibration

1 Introduction

The main focus of this research is friction between the tip of a micro-cantilever and a sample surface. Micro-cantilevers are an integral element in Atomic Force Microscopes (AFM), which are used to image surfaces, and measure friction. Tip motion or deflection is a measure of surface topography as well as friction at the tip/surface interface

Tip deflection (or angular tilt) is measured by monitoring the movement of a laser beam that is reflected off of the micro-cantilever tip. In some experiments the micro-cantilever is driven (tapping mode) while in some cases the cantilever is moved across a surface in the contact mode. This study focuses on the motions of the cantilever and the interactive forces while in the contact mode. In general the tip of the micro-cantilever beam can move in a vertical plane with two degrees of freedom. It is assumed that the cantilever tip is driven by the Lennard-Jones force, between the nearest atom on the tip of the micro-cantilever to a row of atoms on a surface, which moves, at a constant velocity under the tip.

Friction studies can be divided into four scale levels.

Macro-Scale Friction	100 μm – above
Micro-Scale Friction	1 μm – 100 μm
Nano-Scale Friction	1 nm – 1 μm
Atomic-Scale Friction	3 Å – 5 Å

This is an arbitrary scale system that is commonly found in literature. The following sections give an overview of state of the art of friction technology within each scale.

Macro-Scale Friction

This section gives a historical background of dry friction and provides a baseline for the main focus of this study. Macro-friction can be broken down into two types static and kinetic, which describes the state of motion of an object such as a box pressed against a rigid plane surface. Static friction is the force that would be required to initiate movement of the box along a plane. Kinetic friction is the force that is required to keep the box in motion as it slides across the surface. Leonardo da Vinci (1452-1519) made the earliest recorded experiments on friction. He observed that friction force was independent of the area of contact and that friction force was proportional to the applied load [1]. Now, friction has usually been quantified by a coefficient of friction, which was defined by the French engineer Amontons in 1699 [2]. He quantified that the coefficient of friction by dividing the friction force by the normal force as seen below.

$$f = \frac{\text{Friction Force}}{\text{Normal Force}} \quad (1)$$

Coulomb's theory of friction states that friction is due to the interlocking of surface asperities, and that friction is a representation of the work required to lift the load over the asperities. For sufficiently rough surfaces this is generally accurate. This is not necessarily true for smoother surfaces for which molecular adhesion contributes to friction due to attractive and repulsive forces between molecules. There is a set of historical laws that pertain to dry friction based on Amontons and Coulomb [2].

- Friction force is proportional to the applied load.
- Friction is independent of gross area of contact between surfaces.
- Friction depends on the nature of the sliding surfaces.
- Friction is independent of the sliding velocity.

The coefficient of friction as described above is our current fundamental understanding of friction, which is widely used and taught to most engineers there are several examples in

Table 1. Currently there is a good understanding of micro-scale friction, but there is research still being done in micro-scale, nano-scale, and atomic scale friction to get a better fundamental understanding of friction at these levels. This is not the only theory as to the source of friction.

In 1929 Tomlinson [3] presented a hypothesis explaining dry friction based on molecular interaction. He recognized that molecular or atomic interactive forces exist between two molecules and that these forces have both attractive and repulsive components. Molecules are in static equilibrium at a separation distance when the attractive and repulsive forces are equal. He suggested this equilibrium distance is about 3×10^{-8} cm, which is equal to 0.3 nm ($3\text{\AA}$). However, when the molecules move they impact each other and the repulsive force between them causes them to separate. According to Tomlinson's hypothesis, during this impact and separation, heat is generated, energy is lost and this lost energy is manifested as mechanical friction. This intermittent molecular contact takes place across the apparent area of contact producing friction across the contact surface.

Tomlinson also suggested that friction can be related to the elastic constants of the materials in contact and presented the following friction formula.

$$f = 1.07 \times 10^4 [\theta_I + \theta_{II}]^{2/3} \quad (2)$$

where θ_I and θ_{II} are derived from the following equation for molecules I and II.

$$\theta = \frac{3E + 4G}{G[3E + G]} \quad (3)$$

E is Young's modulus and G is the shear modulus.

Table 1: Tomlinson's results for the coefficient of "Dry" static friction [2].

Values for Material on Material			
Hard Steel	0.39	Brass	0.63
Mild Steel	0.41	Aluminum	0.94
Platinum	0.45	Glass	0.94
Nickel	0.39	Tin	1.11
Copper	0.60	Lead	0.39-3.30

Bowden and Tabor [4] point out that when two surfaces are brought together under a load, there is a difference between the real area of contact and the apparent area of contact. The apparent area of contact is based on the overall dimensions of the mating surfaces. The real area of contact is the sum of the actual contact areas between the microscopic peaks of the irregularities of the surface. These pioneers in surface science show that the real area of contact increases directly with the applied normal load and is independent from the apparent area of contact. The real area of contact varies inversely with the yield pressure, which is approximately equal to three (3) times the elastic limit of the softer material. Their work explains why friction is independent of the apparent area of contact.

Friction is also believed to be the forming, breaking, and reforming of welds between surfaces when a load is applied. The actual area carrying the load along the surface is a fraction of the gross surface area because even the smoothest surface is not truly flat on the molecular level, and this area is proportional to the applied load. The higher the load the larger the actual contact area, and if the load is reduced, so is the actual contact area. If the contact area is small there are high stresses being carried therefore the surfaces weld together. The contact stress for the net areas seems to be independent of the applied load, because as the load increase the net area increases. This leads to the stick-slip action of welding and breaking of welds between surfaces, which happen in a very brief time.

Thick Film Lubrication

Early testing by Tower [5, 6] showed that two bearing surfaces can be separated by a thin film of liquid under certain operating conditions of load, speed, and viscosity. He measured film pressure distributions around journal bearings and concluded that this pressure is great enough to support bearing loads. Reynolds [7] applied the principles of fluid mechanics to formulate differential equations, which predict fluid film pressure distributions. This pioneering work of both Tabor and Reynolds [2,8] established the

foundation for analytical advances, which has provided a sound basis for the practical engineering design of thick film lubricated bearings.

Three types of thick film lubricated bearing are: hydrodynamic, hydrostatic and squeeze films. Hydrodynamic bearings require sliding motion between bearing surfaces. Examples here are journal bearings and slider bearings. Hydrostatic bearings rely on external pumps for fluid film pressure. In this case, fluid is circulated through bearings at specified pressure and flow rate for establishing and maintaining a specified operating film thickness. Squeeze films generate their film pressure from the squeezing motion of two approaching bearing surfaces. Pressure builds in the fluid because the fluid cannot be squeezed out instantaneously. Pressure distribution in the film depends on shape and size of the bearing.

If properly designed and maintained, all three types of bearings would experience no wear. Some bearings of these types have operated over a period of 30 years with no measurable wear. Friction generated heat and temperature are important considerations in design.

Film thickness in hydrodynamic bearings varies from application to application. Listed below are a few numbers for reference.

- * Large steel shafts running in babbitt bearings (turbo generators, fans, etc.) – 0.003 to 0.005 in. (0.076 to 0.13 mm)
- * Small, rigid automotive and aviation engine bearings, with very finely finished surfaces, - 0.0001 to 0.002 in. (0.0025 to 0.005 mm)

The coefficient of friction for hydrodynamic lubricated bearings may be as low as 0.001 or even less. The actual value depends on: lubricant viscosity, rotational speed and bearing load. The relations between coefficient of friction and these key operating parameters were first graphically display by McKee [9] see Figure 1. In Figure 1 the symbols represent the following Z is the viscosity, N is the rotational speed, and p is the pressure applied to the bearing.

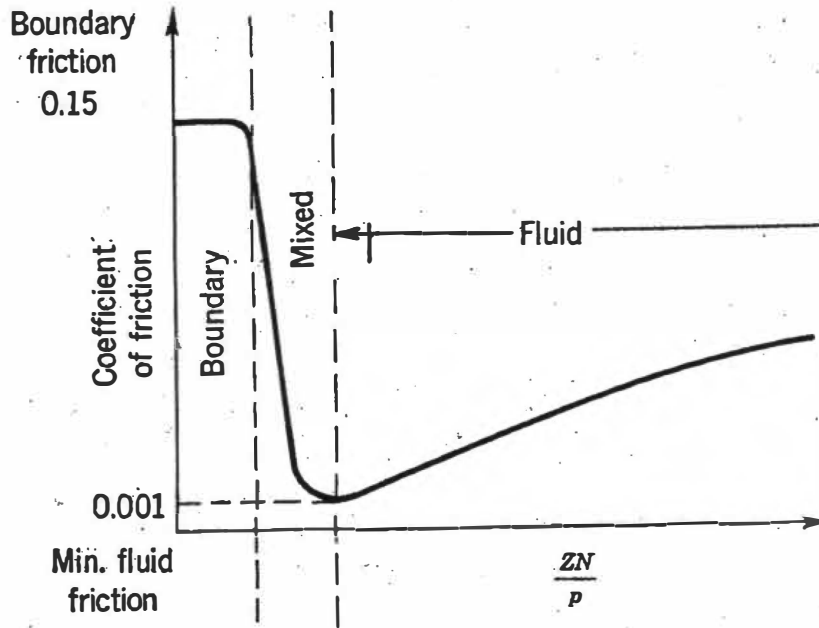


Figure 1: Plot of Coefficient of Friction versus zN/P , or McKee Plot [9].

An experiment was designed and conducted by Karelitz [10] for the purpose of determining the lowest practical limit for fluid film lubricated bearings. Using high quality smooth bearing materials, one would find that the minimum film thickness could reach levels as low as 0.00005 in. (approx. 1 μm). Measurements of surface asperities showed that the peak to valley distances of the asperities were the same order of magnitude as the experimentally determined minimum film thickness. This observation is in agreement with work conducted by McKee [11].

Boundary Lubrication

Boundary lubrication is defined as a condition in which the fluid film does not separate the surfaces greater than the distance equal to surface roughness. Under this condition, the surfaces come into intermittent contact with the microscopic peaks on each surface and the bearing surfaces are separated by a few layers of fluid molecules. Under this condition, friction and heat increase drastically. The bearing usually gets hot and the surfaces seize together.

Surface finish is known to have a direct effect on friction under boundary lubrication conditions. To alleviate heat generation, surface roughness may be honed to a fine level or the bearings may be broken in at lower than operating speeds.

McKee [9] conducted tests on journal bearings and showed how operating conditions and surface roughness affect coefficient of friction seen in Figure 1. His data shows that under certain conditions the friction can be minimized. To the right of the minimum point, bearings operate under thick film conditions. Under these conditions, the bearing has established a constant operating temperature. If the load on the bearing is increased, the operating point moves to the left until thermal equilibrium is again established. Additional increases in load will lower the coefficient of friction until the minimum point has been reached. Further increases in load will cause boundary film lubrication causing the friction and heat to increase. The bearing quickly fails when this happens.

Fuller [2] discusses four regions of bearing behavior in Figure 1.

- 1) Thick film region – Bearing surfaces are completely separated by a liquid film. When the lubricant is free of abrasive particles, wear is prevented. The coefficient of friction is as low as 0.001 or less.
- 2) Thin film lubrication region – This region represents the lower limit of complete separation by a film. Film thickness varies from around 0.0002 in. down to 0.00005 in. Bearing rigidity and surface smoothness are important. Some tests [12] indicate that local fluid properties differ from bulk properties of the lubricant.
- 3) Mixed film region – Loading is so severe that complete surface separation cannot be achieved by the lubricant. Most of the surface experiences rubbing without the benefit of complete separation of the peaks and valleys of the surface roughness. At best, lubrication is achieved by surface separation by a few layers of fluid molecules. The coefficient of friction under this condition may range from 0.02 – 0.08.

- 4) Boundary film region – There is no fluid film because of either low viscosity or velocity or because of high bearing load. Film thickness can only be described in terms of molecules. The coefficient of friction may range between, say, 0.08 and 0.14.

Two factors can move the minimum friction point to the left. One is surface smoothness and the other is the “oiliness” of the lubricant. Surface smoothness is sometimes achieved by “running in” bearings, i.e., initially running a new machine at lower than specified operating speeds. This allows the bearing surfaces to polish themselves to some extent. The second factor is that some lubricants stick to surfaces better than others and are able to maintain wet ability under extreme rubbing conditions. The “oiliness” effect on friction is illustrated Figure 2. Figure 2 shows the change in friction for different lubricants for the dimensionless parameter ZN/P . Where Z is the viscosity, N is the rotational speed of the bearing, and P is the pressure on the bearing.

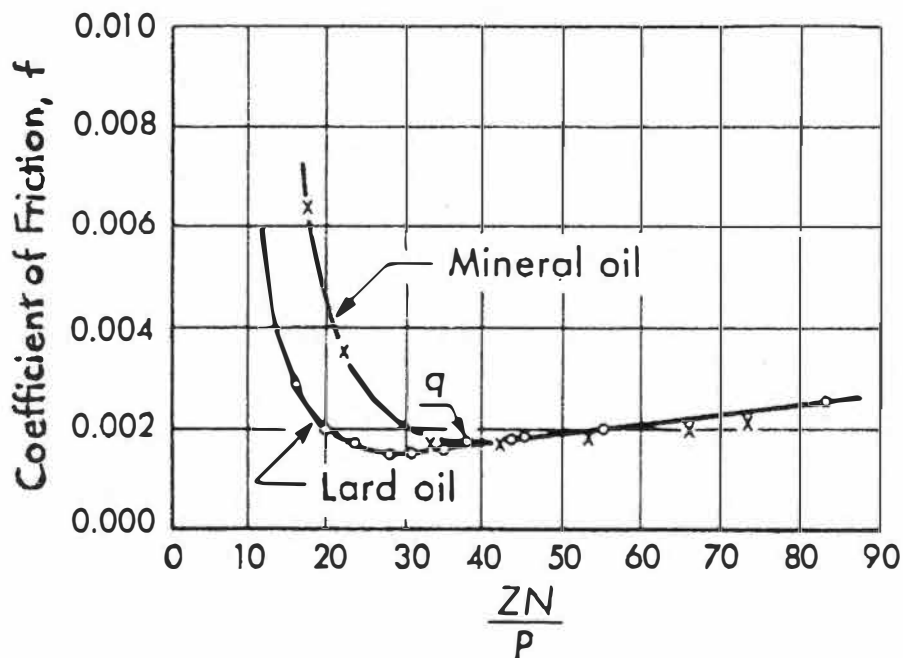


Figure 2: Effect of Oiliness on Bearing Performance [13].

Sleeve Bearings

Sleeve bearings are simply a journal (usually part of the shaft) and a sleeve (or bearing). Many times there is no lubricant. The sleeve is made of some type of low friction material, such as Teflon ($f = 0.1$). In this case the load or bearing pressure, as well as the rotary speed, is small. When the sleeve wears out it is simply replaced. These types of bearing are commonly found in household appliances.

Rolling Contact Bearings

Ball bearings and cylindrical roller bearings are classified as rolling contact bearings. Other machine elements such as gears and cams can also contain rolling/sliding contact surfaces. The load capacities of these types are cataloged by vendors. So the choice here is to select bearing size and type to accommodate a specified load and speed to give a specified level of reliability.

Advantages of rolling contact bearing over thick film lubricated bearings are simplicity and reliability of design. Ball bearings, for example, can still function even though they may have established a defect during operation. On the other hand, hydrostatic bearings can be designed to support football stadiums with minimal space in comparison to ball bearings.

Angular contact ball bearings are typically found in automobiles and everyday appliances. Rotary speeds range up to about 2000 rpm. They also find special application in aircraft gas turbine engines where shaft speeds are in the range of 15,000 to 30,000 rpm. These bearings are also used in the turbo pump of the main engine of the space shuttle, which operate at speeds near 80,000 rpm. In both cases, lubrication in the Hertzian contact region is essential.

Overall friction coefficient in rolling contact bearings is about 0.01. About 60 % of this friction force is caused by moving the ball and its cage through the lubricant. Only 20 % is consumed in micro slippage between ball and race. Friction and heat generation are affected by the coefficient of traction associated with micro slippage within the Hertzian contact region [14].

The fluid dynamics including friction within the Hertzian contact region is a specialized area called elasto-hydrodynamic lubrication (EHL). Here the analysis includes surface deformations and changes in fluid properties, which are caused by extreme contact pressure. Typical surface finish on the balls and races is about 20 μm in. Minimum film thickness is roughly 1 μm [15].

Comparison of Coefficients of Friction

Table 2 shows the range of coefficients of friction common to macroscopic engineering machine elements. The numbers give a baseline reference for coefficients of friction in micro-electro mechanical systems.

Micro-Scale and Nano-Scale Friction

Ruan and Bhushan [17] suggest that micro-scale friction in an AFM is not caused by the atomic-scale stick-slip process, but by the variations in lateral forces between the sample and the probe tip. This study found that there is a correlation between the local slope of the surface and variations in friction suggesting that a ratchet mechanism is the cause of micro-scale friction. That was initially proposed by K. R. Makinson [18] and later discussed by D. Tabor [19]. Evidence of the ratchet mechanism can be seen in surface roughness profiles and the corresponding friction profiles.

Atomic forces at the micro. and nano-scale are due to the molecular interaction between atoms. The main atomic forces being examined in this study are the attractive and repulsive forces between atoms. The attractive forces are also called atomic adhesion, which are due to capillary and atomic forces. Atomic adhesion can be shown by measuring the tip deflection of the micro-cantilever beam as it is moved straight down toward the surface. When the tip of the micro-cantilever gets close enough to the surface the tip is pulled down into the surface. The cantilever beam is then moved down past the point of contact with the surface. Then the cantilever is moved up away from the surface.

Table 2: Comparison of friction [16].

	Coefficient of Friction (Typical)
Dry Friction	
Generic	0.3
Steel on Copper	0.15
Teflon on anything	0.1
Thick Film Bearings	
Journal Bearings	0.001
Slider Bearings	0.001
Boundary Films	0.15
Sleeve Bearings	0.1
Roller Contact Bearings	0.002

The tip of the micro-cantilever sticks to the surface as the micro-cantilever beam is moved up from the surface until the spring force in the cantilever beam is strong enough to overcome the attractive atomic forces. At this point the tip of the micro-cantilever beam comes loose from the surface, and moves back to the non-deflected position [20]. This can be seen in the Figure 3, which is a force-distance curve for the contact between the cantilever tip and the surface [20]. Note that point B is where the tip is pulled down into the surface due to the attractive forces from the zero deflection point A. Point C is where the cantilever becomes unstuck from the atomic adhesion when it is being moved away from the surface.

Adhesion is a force between the tip of the micro-cantilever and the surface. This force will be modeled using the Lennard-Jones potential, which is discussed later in greater detail. The bond forces, which holds the atoms together are being neglected in this study along with chemical reactions.

Electrostatic forces are due to the positively and negatively charges on the surface causing attraction or repulsive forces.

Capillary surface forces lead to an increase in the adhesive force on the tip of the micro-cantilever beam due to meniscus forces. These are due to the development of meniscus bridges between the surface and the cantilever tip created by moisture in the air.

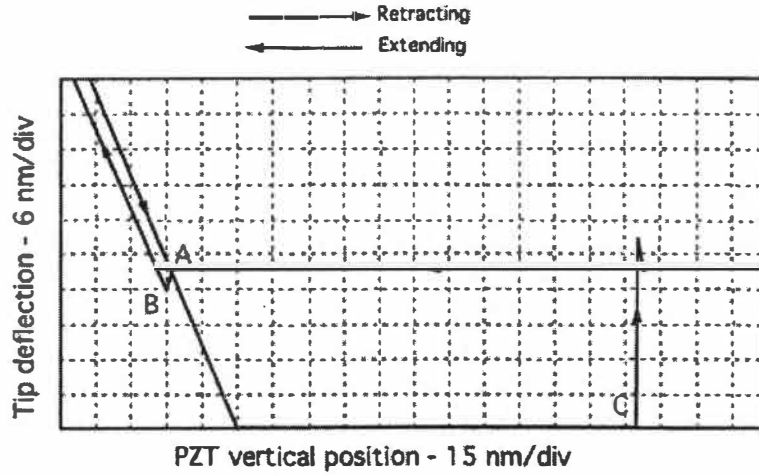


Figure 3: Typical force-distance curve for a contact between the cantilever tip and the surface from [20].

These forces depend on the size of the tip of the micro-cantilever and the relative humidity. As the humidity increases the adhesive forces increase; low humidity has no real effect on the adhesion of the micro-cantilever tip. Figure 4 shows plots of the adhesive forces and the coefficient of friction due to capillary forces and tip diameter for Si (100) [20].

Control of Friction at the Micro-Scale

Friction magnitude and the propensity for stick-slip type friction has been the focus of recent studies. One study [21] showed that friction response can be altered by inducing shear within a mixed lubricant monolayer of base solvent and an additive. This combination makes it possible to alter friction magnitudes and to achieve smooth sliding friction at low sliding velocities.

Braiman's [22] analytical modeling of a nano-array of atoms within and at surface interfaces, shows that mechanical vibrations can cause a shape reduction in friction when the amplitude of vibration reaches a critical threshold.

Gao, Jianping, W. D. Luedtke, and Uzi Landman [23] investigate mechanisms of modifying, controlling, and reducing friction in thin-film boundary lubricants through molecular dynamics simulations.

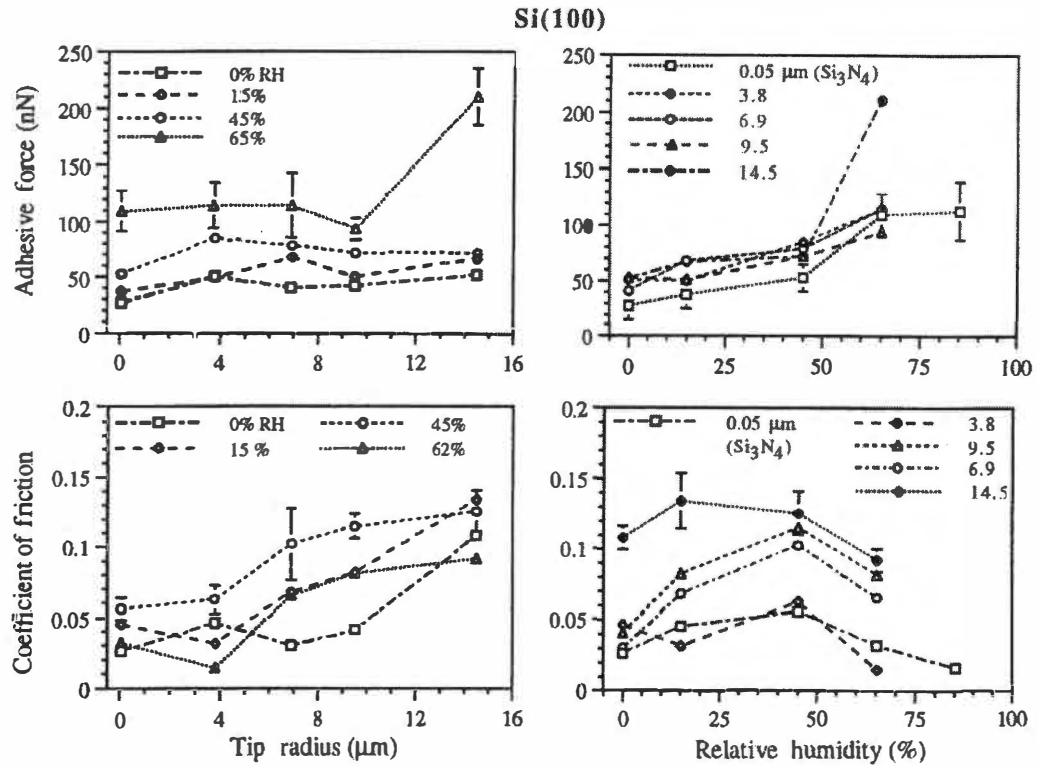


Figure 4: Adhesion and friction coefficient influenced by capillary forces based on relative humidity and tip size [20].

The study shows that friction can be controlled (reduced) by imposing transverse mechanical oscillations of small amplitudes (about 1 angstrom) on the bearing surfaces. The vibrations tend to frustrate the ordering of the film and thus reduce fluid drag to the bearing surfaces.

Drummond and Israelachvili [24] verified this phenomenon experimentally. They state that molecularly thin interfacial films and boundary monolayers can exist in different dynamic “frictional” states depending on sliding velocity, load and temperature. Furthermore, boundary layers can enter a “super-kinetic” state of very low kinetic friction at high sliding velocities.

Atomic Scale Friction

Atomic scale friction is the force associated with the interaction of atoms on a smooth surface, and atoms on another surface such as the tip of a micro-cantilever beam. Atomic scale friction measurements have shown that periodicity of friction profiles

exhibited a similar periodicity as the corresponding topography of the atomic surface [17, 25]. The peaks in the friction profiles are shifted relative to the topography profile high points. Ruan and Bhushan [17] suggest that the stick-slip process does not cause the periodicity variations in friction, and that further experimentation is need. The stick-slip process occurs when the tip of the micro-cantilever beam first sticks to the surface during scanning due to the attractive forces, and then slips from the surface. There is a phase difference between friction and atomic surface peaks. This phase difference can be explained analytically through the use of inter-atomic potential based on the Lennard-Jones [26] formulation.

Stick-slip has been observed in measurements at the atomic level [27-30], microscopic and macroscopic levels [31, 32]. Some observed variations in local friction force between sample and micro-cantilever tip are believed to be the result of intrinsic lateral forces and these variations may not be the result of atomic-scale stick-slip [31].

Gnecco, Bennewitz, Gyalog, Loppacher, Bammerlin, Meyer, and Güntherodt [33] in the process of studying the velocity dependence of atomic friction studied the “static” atomic potential between the tip of the micro-cantilever beam and a row of atoms acting as a surface as seen in Figure 5. The horizontal “static” energy potential of the tip of the micro-cantilever beam can be seen in Figure 6, which is based on the following:

$$V_{\text{tot}} = V(X_T) + \frac{K_{\text{eff}}}{2} (X_T - X_S)^2 \quad (4)$$

$$V(X_T) = \frac{E_0}{2} \cos\left(\frac{2\pi x}{a}\right) \quad (5)$$

where

$$E_0 = 0.165 \text{ eV}$$

$$a = 0.4 \text{ nm}$$

$$K_{\text{eff}} = 0.86 \text{ N/m}$$

In the second term of Equation 4, X_T and X_S are the tip position and the microscope support position. The second term is the energy stored in the cantilever. The first term is assumed to be a cosine function with initial amplitude E_0 and period a . The reflected energy barrier between two atoms is E_0 , and “ a ” is the spacing between atoms.

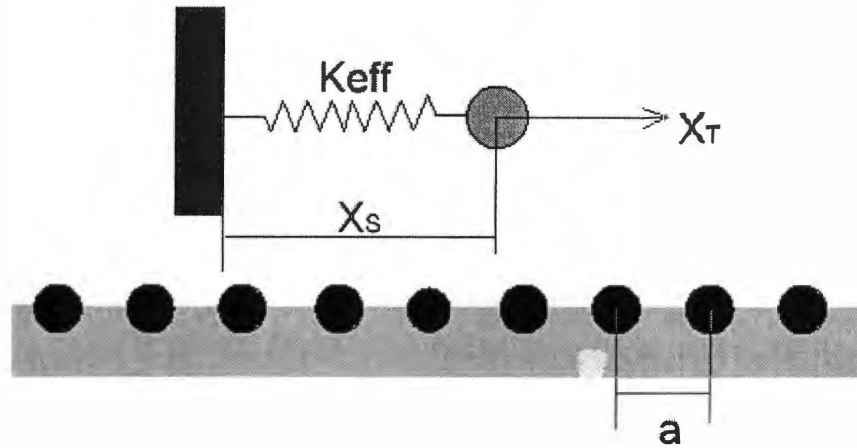


Figure 5: Sketch of the system modeled using Equations 4 and 5.

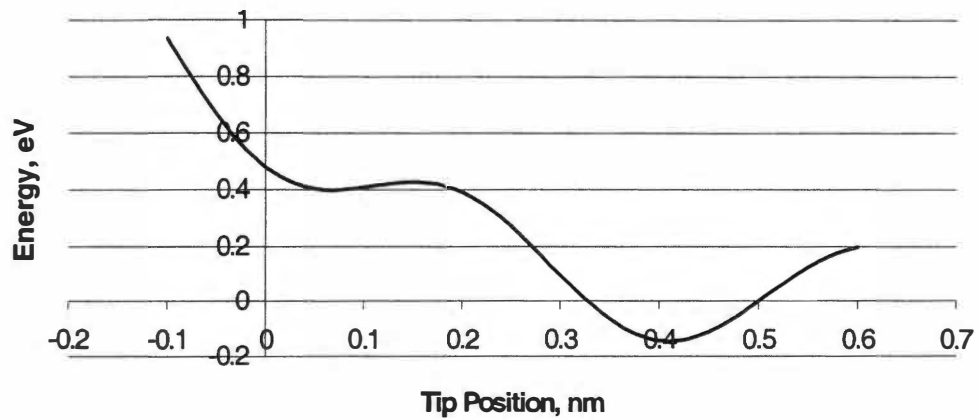


Figure 6: Potential energy recalculated based on Gennco [33].

Figure 6 is a plot of the potential energy of the system according to Equation 4. The plot shows three equilibrium positions, two of which are stable and one being unstable. The derivative of the potential energy of the system is [33]:

$$\frac{dV}{dx} = K_{\text{eff}}(X_T - X_S) - \frac{E_0}{2} \frac{2\pi}{a} \sin\left(\frac{2\pi x}{a}\right) \quad (6)$$

The force, which is the derivative of the potential energy, is plotted in Figure 7. This force represents the force that is required to move the tip (atom) horizontally over a row of atoms. This force plot shows that a positive force is required to move the tip forward and out of the first stable equilibrium position. Once the tip reaches the second equilibrium position (unstable) the tip slides, forward to the third and stable equilibrium position. This plot was used by the authors of [33] to explain how stick-slip friction might be created at the atomic level.

The Atomic Force Microscope (AFM)

Laboratory equipment is available to image surfaces, and obtain friction data at the micro, nano, and atomic-scale. The surface force apparatus (SFA) was developed in the 1960's, and is used to study static and dynamic properties of a thin film between two smooth surfaces. The scanning tunneling microscope (STM) was developed in 1982, and

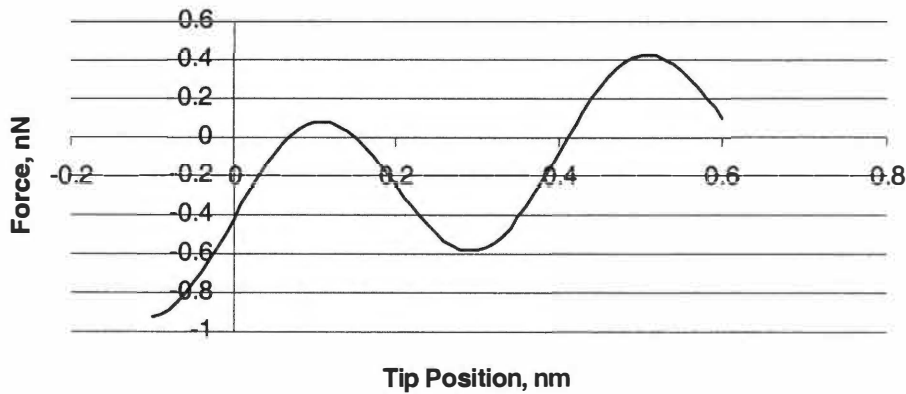


Figure 7: Atomic force which is the numerical derivative of the potential energy based on Gennco [33].

is used to image clean surfaces and even lubricant molecules. It works for electrically conductive materials and is capable of atomic resolution.

The atomic force microscope (AFM), which was developed in 1985 by Gerd Binnig [20], is capable of producing high-resolution Three-Dimensional images of the surfaces. It can also measure a very small force less than 1 nN. The AFM (See Figure 8) determines these small forces by detecting the motion of a flexible cantilever, which has a very small mass. The sample surface is moved under the cantilever instead of the cantilever's moving over the surface. If the cantilever were moving, it would introduce vibrations due to the motion of its support structure. The cantilever beam spring constant must be less than the atomic spring constant to be able to get atomic resolution. The cantilever beam has a small tip on the end of it, and must be as sharp as possible. If the tip is not sharp the imaging resolution will drop.

The development of the atomic force microscope led to the development of the friction force microscope (FFM) or the lateral force microscope (LFM). This apparatus can be used to measure the lateral or friction force along with investigation fabrication/machining, wear, and indentations [20]. Table 3 has some of the typical operating parameters for SFM, STM, and AFM/FFM.

How do AFM and FFM image surfaces and measure friction? The way an AFM and FFM measures changes in the position of the micro-cantilever beams is by using a laser beam. The laser beam is generated by a laser diode. The beam is sent through a prism, which directs the beam at the free end of the micro-cantilever at an angle of about 10 degrees from the horizontal. The laser beam is reflected off the micro-cantilever beam to a mirror, which redirects the beam to four photo detectors. The photo detectors give the AFM the sensitivity to measure the deflection of the micro-cantilever beam. The top and bottom photo detectors measure the vertical deflection of the micro-cantilever beam. The way the AFM measures friction is using the other two horizontal photo detectors. These detectors measure the twisting of the micro-cantilever beam, which is caused by friction or lateral forces acting on the micro-cantilever beam's tip. Ruan and Bhushan developed a procedure to minimize the error in the friction measurements by measuring the friction in two opposite directions, and subtracting the difference between the two [20].

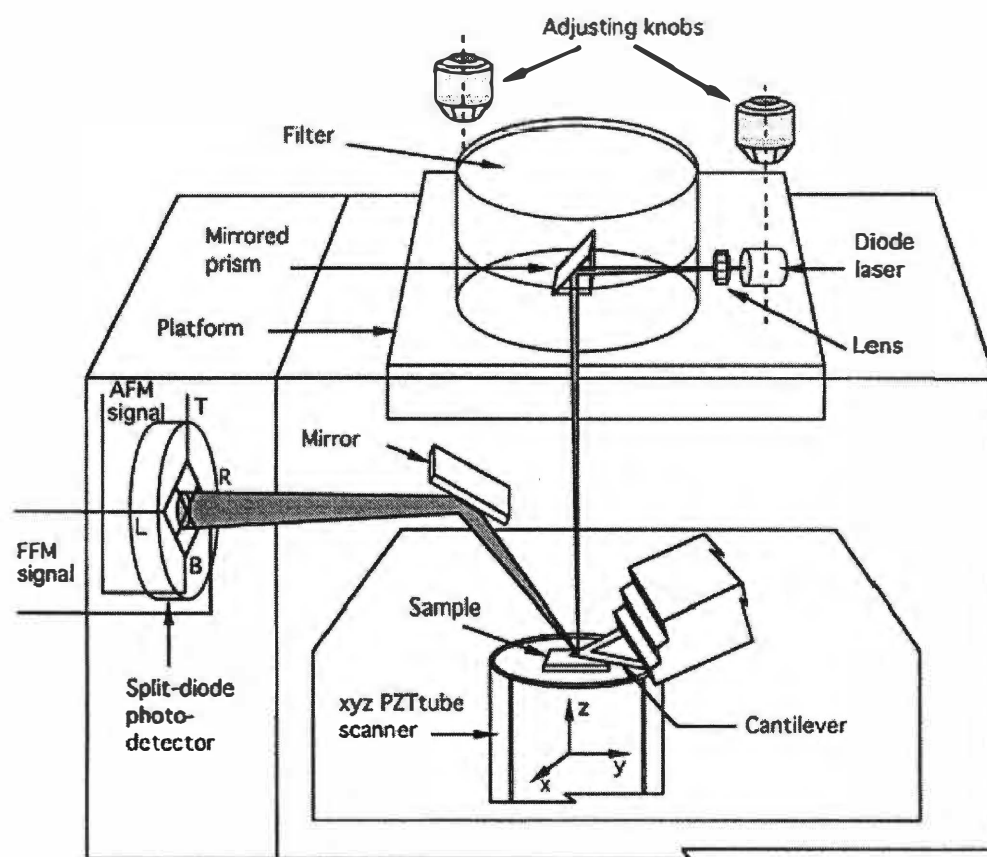


Figure 8: Atomic Force Microscope and Friction Force Microscope (AFM/FFM) from [20].

Table 3: Typical Operating Parameters for SFA, STM, and AFM/FFM used in micro. and nanotribological studies [20].

Operating Parameter	SFA	STM*	AFM/FFM
Radius of mating surface/tip	~10 mm	5-100 nm	5-100 nm
Radius of contact area	10-40 μm	N/A	0.05-0.5 nm
Normal load	10-100mN	N/A	<0.1 nN-500 nN
Sliding velocity	0.001-100 $\mu\text{m/s}$	0.02-2 $\mu\text{m/s}$ (scan size ~ 1 nm x 1 nm to 125 μm ; rate < 1-122 Hz)	0.02-2 $\mu\text{m/s}$ (scan size ~ 1 nm x 125 μm ; scan rate <1-122 Hz)
Sample limitations	Typically atomically-smooth, optically transparent mica; opaque ceramic, smooth surfaces can also be used	Electrically- conducting samples	None

*Can only be used for atomic-scale imaging.

The micro-cantilever beam is the main component in the AFM. The micro-cantilever beams are usually on the order of 300 micro-meters in length, 30 micro-meters in width, and 1 micro-meter in thickness. The tip of the micro-cantilever is its major component because the shape of the tip affects how the micro-cantilever interacts with the surface, which is the basic determinant of the resolution of the microscope. The higher the resolution, the better things at the atomic-scale can be imaged.

There are two basic modes of operation for an AFM, and these are tapping mode and contact mode. Tapping mode is when the micro-cantilever tip is moving up and down, only coming into momentary contact with the surface as it moves under the micro-cantilever. Contact mode is when the micro-cantilever tip is in constant contact with the surface as the surface moves under the micro-cantilever beam.

The atomic force microscope or AFM makes it possible to image surfaces at the nano-scale, and to measure friction. The AFM can also measure friction at the nano-scale. An AFM was used to determine the contour of a surface, and the friction was measured in milli-volt output between the AFM and the surface. Both are shown below in Figure 9.

Opportunity to Improve Understanding of Friction

Friction is a major consideration in designing and building machines. Friction will cause wear on any machine's part. If the friction is great enough, it can cause the machine to shut down or fail. This is true for large machines and small machines such as tires on a car or the spindle of a compact disc player. Currently, friction can be modeled and predicted at the macro-level and even at the micro-level. However, this is not true for the friction at the atomic scale. Friction is a force that causes energy losses, which results in heat generation, reduction in fluid flow in pipes, and wear. The key to knowing how friction affects a design is to know how friction acts, and being able to describe it. Currently the friction at the nano. and atomic-scale can be measured using an atomic force microscope, which measures the friction between a micro-cantilever beam and a smooth surface as one is moved relative to the other.

Predicting the friction is important in order to be able to design micro-

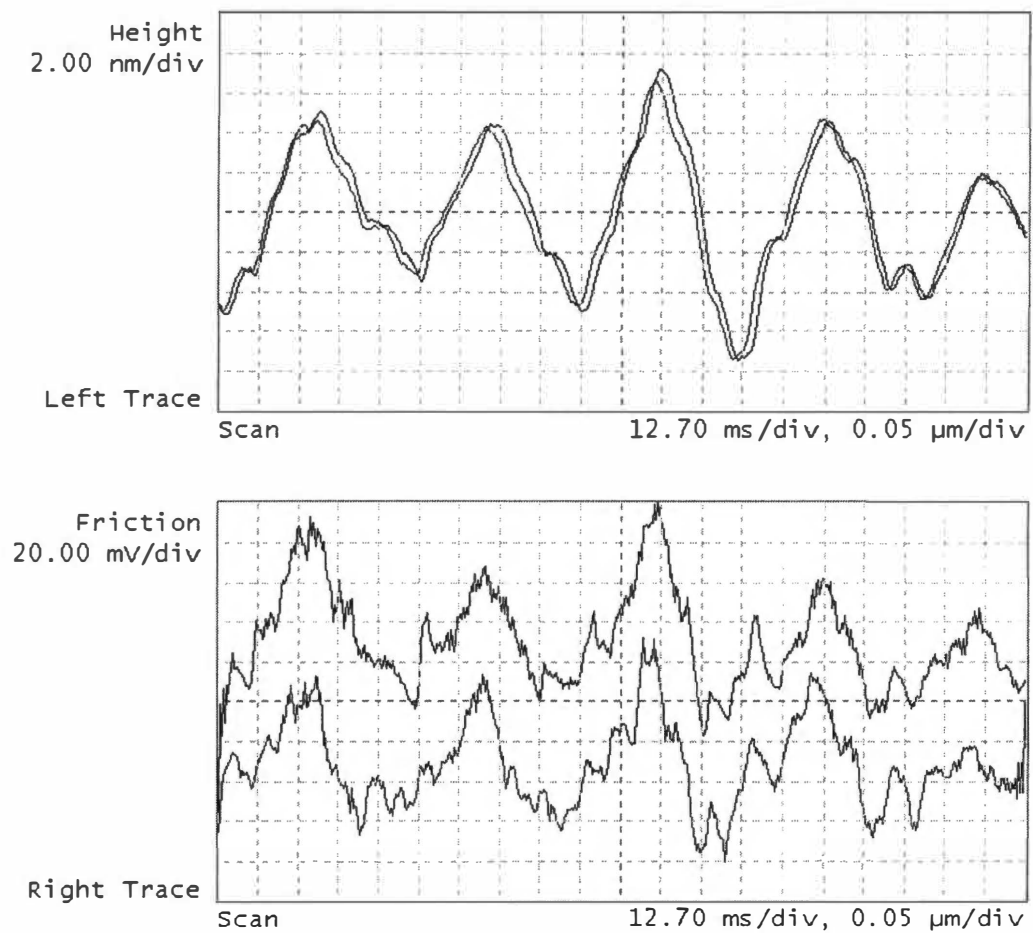


Figure 9: The above plots are examples of data that can be obtained using an FFM [34].

electromechanical devices (MEM). A better understanding is needed of how the friction interacts with the mechanical parts of these MEM devices. Friction will have the same effect, if not more, on these small devices that it would have on any macro-scale device. This is true whether the interaction involves two surfaces, fluids, or fluids and surfaces. It is necessary to be able to predict the friction at this scale in order to design Micro-Electro-Mechanical Machines (MEMS) or Nano-Mechanical Devices. In these designs atomic and nano-scale friction are important because these are the major forces acting on a machine of this scale.

For example, suppose that a device being designed were less than a 100 nm in size and had to have a bearing for a shaft that was 10 nm in diameter. The design of the bearing would require being able to predict the friction at the atomic scale because the spacing between atoms is typically between 0.3-0.4 nm. There would only be a couple of hundred atoms on the surface of the shaft or on the bearing. So the main forces acting on the shaft and the bearing would mainly be atomic forces. This is why a better understanding of friction and atomic forces is needed. The friction will cause resistance to motion in the bearing, but the atomic force acting on the shaft and bearing are important for balancing the shaft, and creating the bearing in the first place. Another good example would be to be able to understand the fundamental mechanics of the micro-cantilever beam, which is used in an atomic force microscope. There is also the need to develop a better understanding of the mechanics of friction at the nano. and atomic scale. Imaging surface and atoms can be improved with a better understanding of the mechanics of the micro-cantilever, because currently it is more a matter of luck, or trial and error, that atoms on a surface can be imaged. With a better understanding of the mechanics involved, better imaging techniques can be developed, so that it may be possible to predict friction at this scale. Currently friction is only measured and not predicted analytically.

It is the goal of this research to improve the understanding of micro-cantilever tip dynamics, and its effect on friction measurements and imaging at the atomic scale. A fundamental understanding of friction at the nano. and atomic scale is required in order for nano. or atomic devices to be designed and built.

2 Objective of Research

The objective of this research is to better understand the mechanisms of friction. This is done by examining the horizontal force component of the forces between one atom on the tip of a micro-cantilever and a single row of atoms lying within an adjacent surface as seen in Figure 10. The model shown in Figure 10 does not include an energy dissipation mechanism between the moving atom on the tip and the surface atoms. The system is conservative and therefore the interactive forces cannot be considered as true friction.

Since the atomic force microscope (AFM) is typically used to measure friction at the atomic and nano-scales, it is also necessary to understand the dynamics of the micro-cantilever tip as it engages a surface. Therefore the focus of this analytical research will be on: 1) tip dynamics 2) related horizontal driving force.

The model assumed in this study is shown in Figure 10. In this simplistic model the grey circle attached to the springs represents an atom on the micro-cantilever tip. The black circles represent the row of atoms modeling the surface. This model will allow the cantilever tip to move in the horizontal and vertical directions as driven by the atomic forces while the surface moves to the left at a surface velocity of V_s . The forces are being modeled using the Lennard-Jones potential. The horizontal driving force is predicted from the motion of the tip and the forces acting on it.

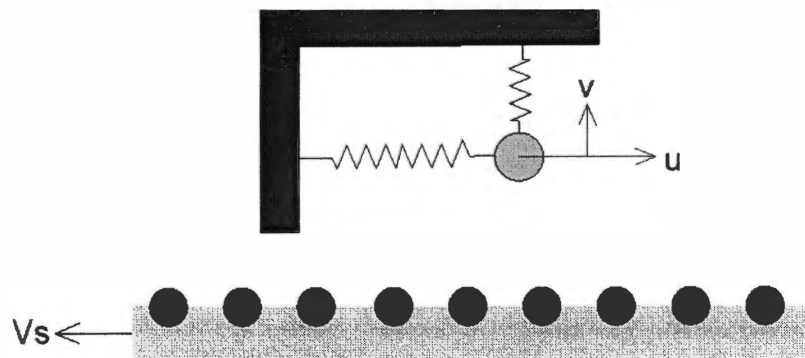


Figure 10: Sketch of the micro-cantilever and surface system.

3 Lennard-Jones Model of the Atomic Potential

Lennard-Jones Potential

In order to be able to model the dynamics and the atomic scale friction of a micro-cantilever beam interacting with atoms on a surface it is necessary to model the atom forces that are acting on the tip of the micro-cantilever beam. There are relationships that have been developed to model the potential energy between atoms based on the distance between atoms. The van der Waals model describes the potential between two surfaces and typically does not contain a repulsive component. The Lennard-Jones potential model does take into account the repulsive and attractive energy between atoms. However, Lennard-Jones is only an approximation of potential energy between two atoms. It is a good approximation for the potential energy between atoms. The Lennard-Jones potential energy model will be used in this study since both the attractive and repulsive components are of interest in modeling the dynamics. These relationships for the potential energy between atoms are the doorway for modeling the atomic force and atomic spring constants between atoms.

The Lennard-Jones potential is an empirical relationship, which uses the distance between two atoms to model the potential energy between two atoms. The Lennard-Jones potential has two forms, one non-dimensional and the other dimensional, as explained by Ashcroft and Mermin [35].

$$\phi(R) = 4\epsilon \left[\left(\frac{\sigma}{R} \right)^{12} - \left(\frac{\sigma}{R} \right)^6 \right] \quad \text{Non-Dimensional} \quad (7)$$

$$\sigma = \left(\frac{B}{A} \right)^{1/6} \quad \epsilon = \frac{A^2}{4B} \quad \text{Non-Dimensional Constants} \quad (8)$$

$$\phi(R) = \frac{B}{R^{12}} - \frac{A}{R^6} \quad \text{Dimensional} \quad (9)$$

$$A = 4\epsilon\sigma^6 \text{ J m}^6 \quad \text{Dimensional Constants} \quad (10)$$

$$B = 4\epsilon\sigma^{12} \text{ J m}^{12} \quad \text{Dimensional Constants} \quad (11)$$

where R is the distance between atoms (m).

The constants sigma (σ) and epsilon (ϵ) are material dependent. They vary between different types of material whether they be solids, liquids, or gases. The material constants sigma and epsilon are used in the non-dimensional form of the Lennard-Jones potential. The units for sigma (σ) are typically in terms of Angstroms or meters (m). The units for epsilon (ϵ) are typically electron volts (eV), Joules (J) or Kelvin (K). The dimensional form of the Lennard-Jones potential use constants A and B . This is the form of the Lennard-Jones potential used in this study. The units for A are either $[\text{J m}^6]$ or $[(\text{nN nm}) \text{nm}^6]$, and the units of B are $[\text{J m}^{12}]$ or $[(\text{nN nm}) \text{nm}^{12}]$. The units used depend on the scale being studied, for example in this study the motion of the micro-cantilever is of interest, and the motion will be on the order of nanometers. Therefore the material constants which are in terms of (nN nm nm^{12}) be used where R is in terms of nm. The Lennard-Jones constants vary with element type as shown in Tables 4 and 5 [35, 36]. The Lennard-Jones constants used in this study are the ones given in the last column.

Table 4: Example of Non-Dimensional material constants used in calculating the Lennard-Jones Potential Function based on information from [35, 36].

	Sigma m	Epsilon J	Sigma Å	Epsilon K	Epsilon eV
Si	3.8260E-10	2.7951E-21	3.826	202.45	2.795E-14
Ne	2.7400E-10	3.1000E-10	2.74	2.2453E+13	0.0031
Ar	3.4000E-10	1.0400E-09	3.40	7.5327E+13	0.0104
Kr	3.6500E-10	1.0400E-09	3.65	7.5327E+13	0.0104
Xe	3.9800E-10	2.0000E-09	3.98	1.4486E+14	0.02
(Used in Research)	3.1623E-10	2.5000E-21	3.16	181.1	2.50E-14

Table 5: Example of Dimensional material constants used in calculating the Lennard-Jones Potential Function based on information from [35, 36].

	A J m ⁶	B J m ¹²	A (nN nm) nm ⁶	B (nN nm) nm ¹²
Si	3.5069E-77	1.1000E-133	3.5069E-05	1.1000E-07
Ne	5.2472E-67	2.2204E-124	5.2472E+05	2.2204E+02
Ar	6.4264E-66	9.9275E-123	6.4264E+06	9.9275E+03
Kr	9.8367E-66	2.3260E-122	9.8367E+06	2.3260E+04
Xe	3.1797E-65	1.2638E-121	3.1797E+07	1.2638E+05
(Used in Research)	1.0000E-77	1.0000E-134	1.0000E-05	1.0000E-08

Potential Energy between Two Atoms

The potential energy between two atoms as seen in Figure 11 is normally defined by the Lennard-Jones potential equation, where the only variable is the change in the distance between atoms. The model is the same whether the atoms are oriented vertically, horizontally, or at some arbitrary angle. The potential energy can be seen as the work required to move one atom relative to another.

Figure 12 below shows how the potential energy changes as the distance between the atoms (R) changes. The potential energy has one equilibrium point, which is a minimum. This point is the point where the attractive and the repulsive energies are equal. As the distance between atoms decreases and approaches zero the potential energy approaches infinity. This is not shown well in Figure 12, but can be proven if the limit of Equation 9 is taken as R approaches zero. It can be shown that by taking the limit of Equation 9 as R goes to infinity, the potential energy will go to zero as shown in Figure 12. Note that the positive term in the Lennard-Jones Equation 9 yields a repulsive force, while the negative term yields an attractive force.

Since this study is done using Cartesian coordinates, Equation 9 can be converted to Cartesian coordinates as seen in Figure 13. The change in horizontal position is the x variable and the change in the vertical position is the y variable as shown below.

$$R = \sqrt{x^2 + y^2} \quad \text{from Equation 9} \quad (12)$$

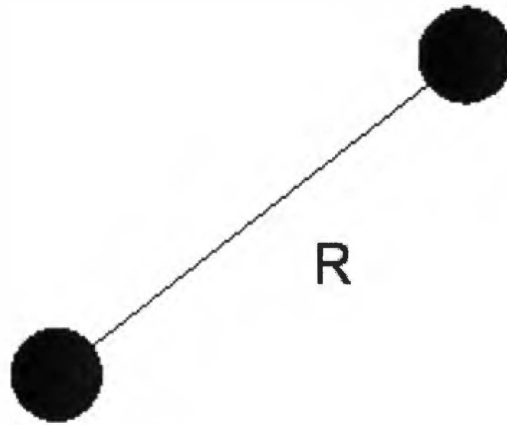


Figure 11: Sketch of two atoms oriented at an arbitrary angle.

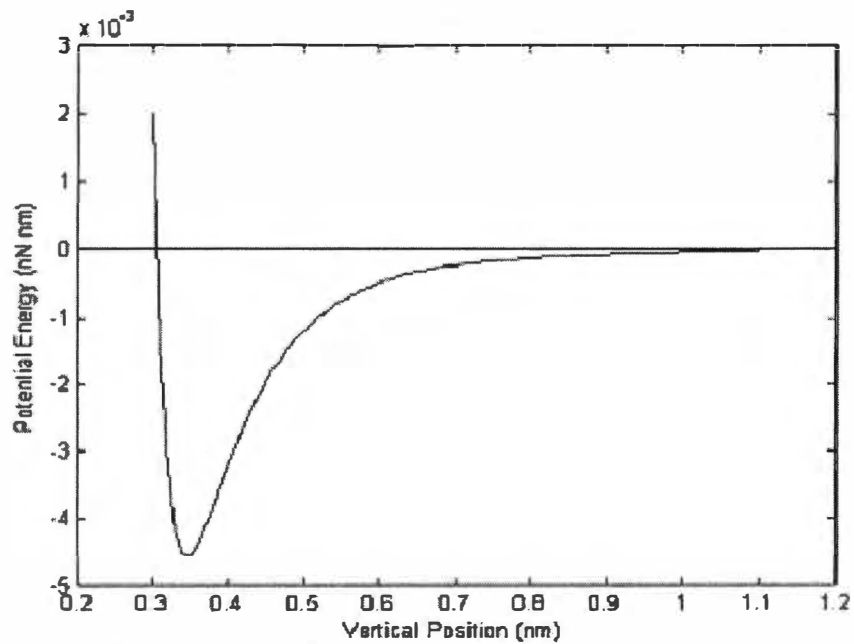


Figure 12: Potential Energy based on the Lennard-Jones Potential between two atoms.
 $A = 1.0\text{E-}5$ (nN nm nm⁶), $B = 1.0\text{E-}8$ (nN nm nm¹²)

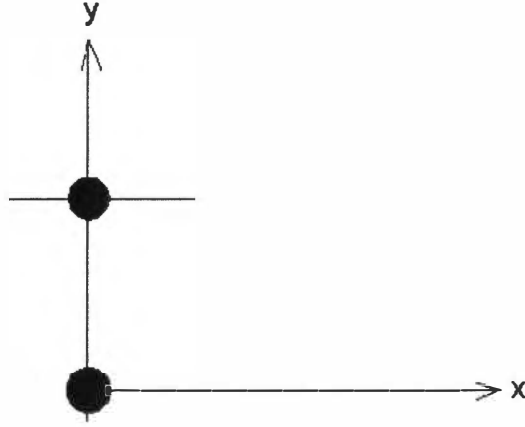


Figure 13: Sketch of two atoms in Cartesian coordinates.

$$\phi(x, y) = \frac{B}{(\sqrt{x^2 + y^2})^{12}} - \frac{A}{(\sqrt{x^2 + y^2})^6} = \frac{B}{(x^2 + y^2)^6} - \frac{A}{(x^2 + y^2)^3} \quad (13)$$

Using these equations, one can see that the results in Figure 12 can be obtained by setting $x = 0$, and letting y varying as seen in Figure 13. In this particular case Equation 14 applies.

$$\phi(y) = \frac{B}{(y)^{12}} - \frac{A}{(y)^6} \quad (14)$$

This is a special case of Equation 13 because it simplifies down to basically the same as equation 9 except that R is now y as shown in equation 14.

Potential Energy between a Single Atom and a Row of Atoms

In this study the tip of the micro-cantilever will be modeled as a single atom. Now to get an idea of the atomic potential between the cantilever tip and the surface, the following model will be used. The model consists of a single atom above a single row of atoms as seen in Figure 14. The easiest way to calculate the potential energy is to use Equation 13. Equation 13 is calculated based on a Cartesian coordinate system. The potential energy $\phi(x, y)$ for this model is an energy field based on x and y .

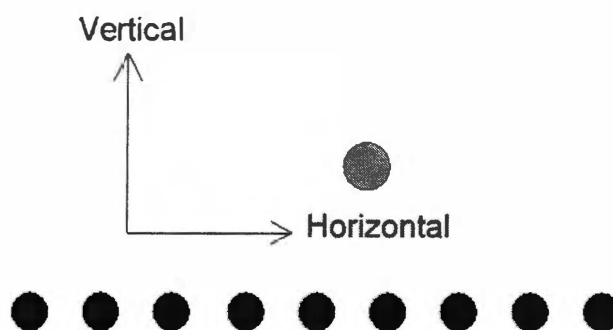


Figure 14: Sketch of a single atom above a row of atoms.

Figure 15 shows the potential energy $\phi(x, y)$ for a single atom above a row of atoms. Examination of the potential energy for a change in the vertical position reveals a pattern similar to that seen in Figure 12. Change in the horizontal position results in a periodic pattern in the potential field. There are several equilibrium points throughout the potential field. These equilibrium points indicate the point where the attractive and repulsive energies are equal. Since the rows of atoms are uniform the equilibrium point is always in between two atoms. The vertical location of the equilibrium point can vary depending on the Lennard-Jones constants used.

How does this relate to the tip of a micro-cantilever beam? The potential field in Figure 15 is potential field for the tip of the micro-cantilever over a row of atoms. This means that in order for the tip to move from one location in the potential field to another there must be a change in energy. This can result in a loss or gain in energy. This atomic potential field $\phi(x, y)$ is the primary driver of tip motion.

Figure 16 is a contour plot for the potential similar to the one in Figure 15, which the contour lines show lines of constant atomic potential energy. The atoms can be easily located on the contour plot where the contour lines are close together. The potential energy decreases as shown in the top of the plot. The contour lines start to level out and are farther apart. In examining Figure 16 the equilibrium points are easily located. They appear as rounded triangle shapes, which have completely enclosed contour.

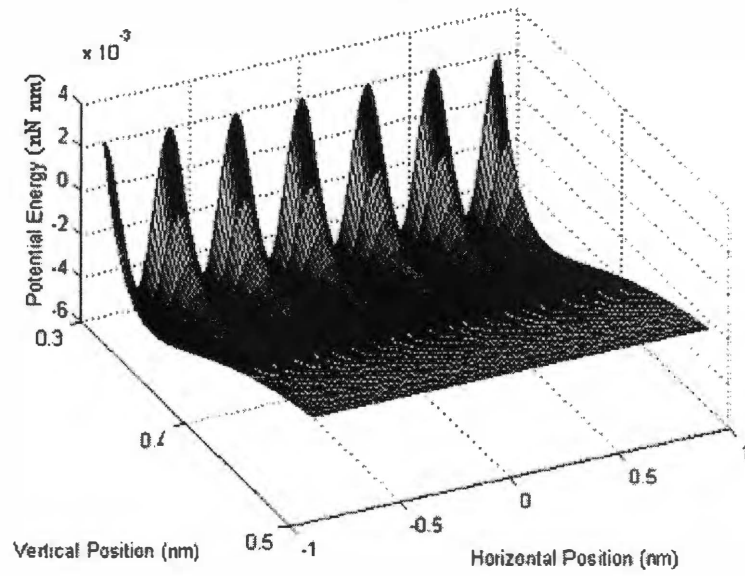


Figure 15: The atomic potential energy field $\phi(x, y)$ between a single atom and a row of atoms.

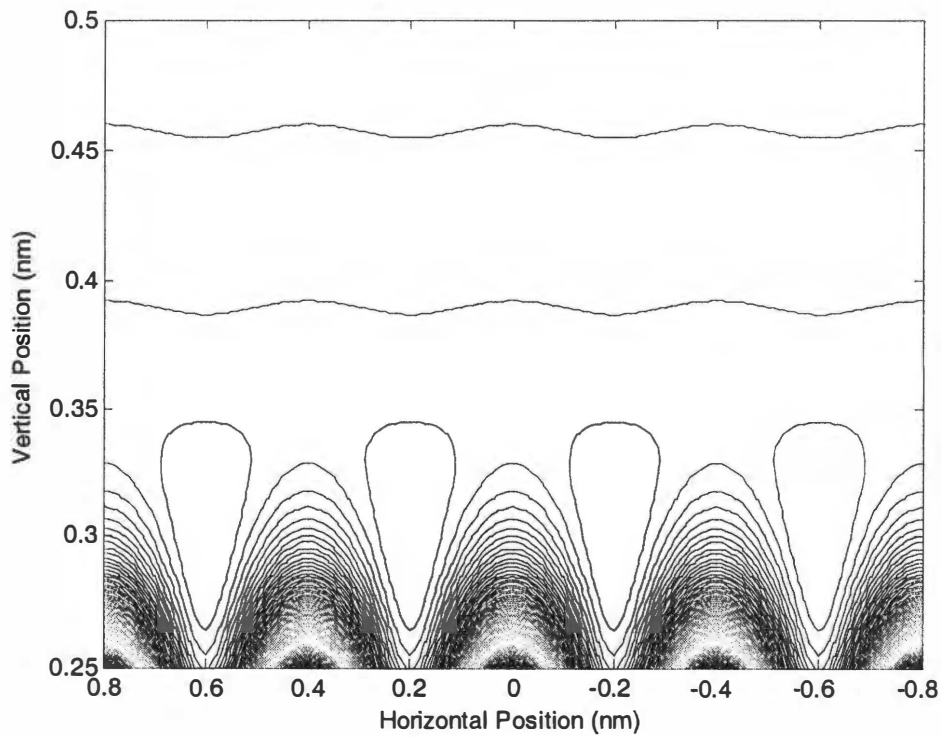


Figure 16: Contour plot showing lines of constant atomic potential energy field $\phi(x, y)$ between a single atom and a row of atoms.

Figure 16 is a contour plot for the potential similar to the one in Figure 15, which the contour lines show lines of constant atomic potential energy. The atoms can be easily located on the contour plot where the contour lines are close together. The potential energy decreases as shown in the top of the plot. The contour lines start to level out and are farther apart. In examining Figure 16 the equilibrium points are easily located. They appear as rounded triangle shapes, which have completely enclosed contour. These contour lines are located in between each atom. All of the other contour lines continue along the surface.

Effects of Springs on the Potential Field

We will now revert to a rectangular coordinate system of u, v as shown in Figure 17. The origin of the u, v coordinate system is the position of the micro-cantilever tip with zero spring load. Since the system being modeled is the tip of a micro-cantilever beam interacting with atoms on the surface, it is necessary to include the potential energy stored in the micro-cantilever. In this study the micro-cantilever will be modeled as a spring/mass system as shown below in Figure 17.

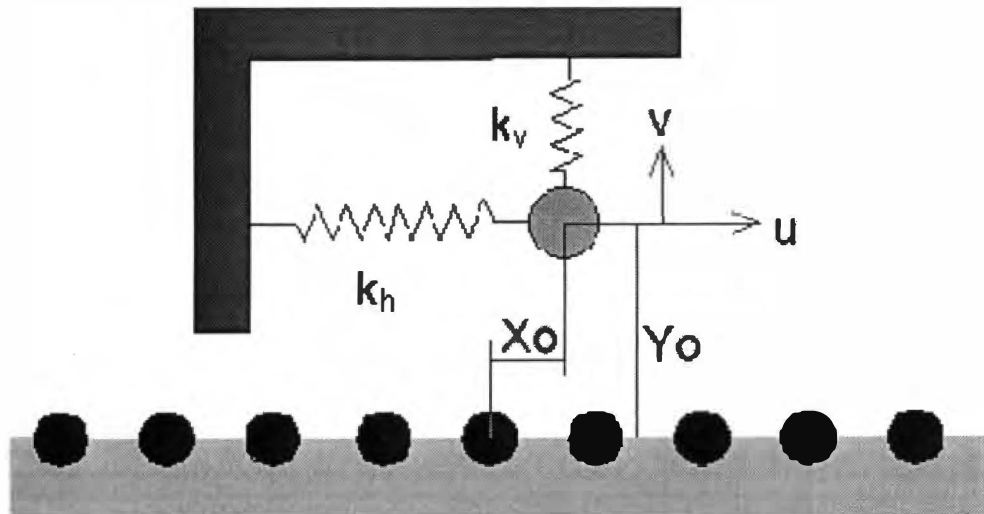


Figure 17: Sketch of the micro-cantilever modeled as a spring mass system over a row of atoms.

The springs will be oriented horizontally, or parallel with the surface, and vertically, or normal to the surface. Assuming small deflections, one can see that the potential energy of the micro-cantilever beam is:

$$\phi_{\text{spring}}(u, v) = \frac{1}{2}(k_h)u^2 + \frac{1}{2}(k_v)v^2 \quad (15)$$

where u and v are the horizontal and vertical changes in the length of the springs from the unstretched position.

The total potential energy in the system is atomic potential energy and the spring's potential energy combined.

$$\phi_{\text{Total}}(u, v) = \phi(u, v) + \phi_{\text{spring}}(u, v) \quad (16)$$

$$\begin{aligned} \phi_{\text{Total}}(u, v) = & \left(\frac{B}{\left(\sqrt{(X_0 + u)^2 + (Y_0 + v)^2} \right)^{12}} - \frac{A}{\left(\sqrt{(X_0 + u)^2 + (Y_0 + v)^2} \right)^6} \right) \\ & + \left(\frac{1}{2}(k_h)u^2 + \frac{1}{2}(k_v)v^2 \right) \end{aligned} \quad (17)$$

This is the total potential energy for the system being modeled. Figure 18 below shows the total potential energy field for the combined atomic potential and the spring's potential energy. The parabolic shape is due to the spring's potential energy, and the rest is due to the atomic potential energy.

Directional Derivatives

What makes the potential energy field useful is that the force required to move through the potential field can be determined. The change in potential energy can be seen as the product of the local force and an incremental displacement, $d\phi = Fdr$. Local force, F , can be determined by taking the derivative of the potential function. Since the change in distance can be arbitrary, let us assume that vector $\hat{r}$ is the arbitrary change in the tip's position in the potential field as seen in Figure 19.

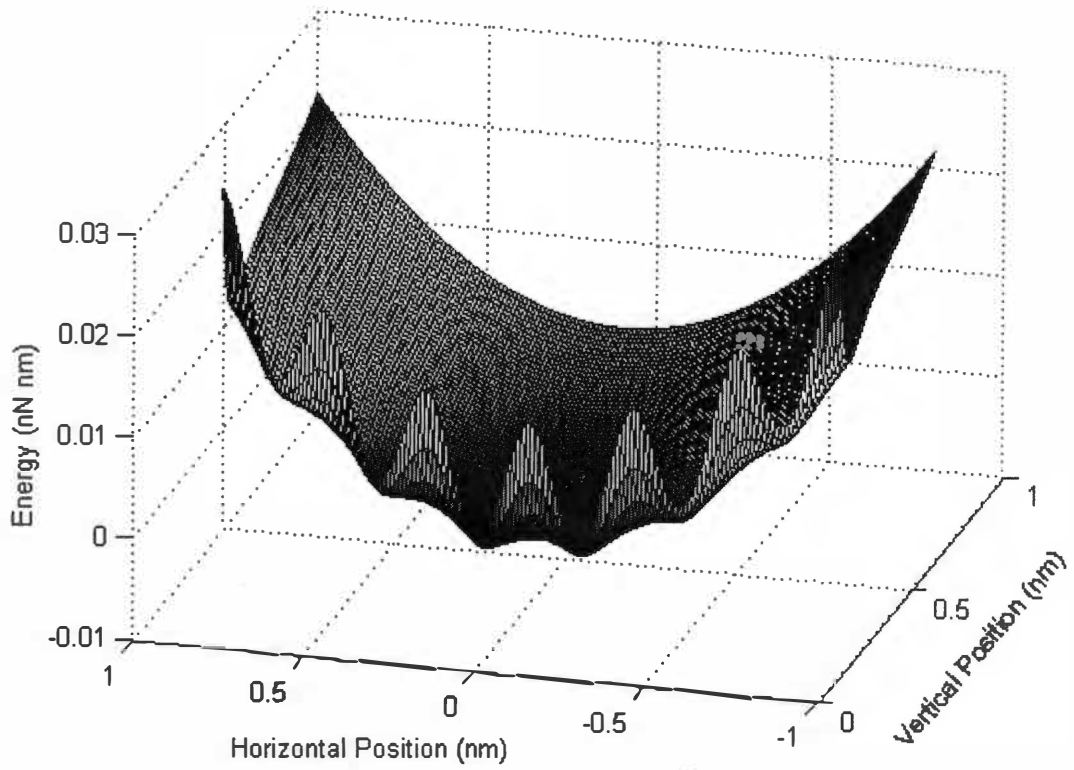


Figure 18: The total potential energy field including spring and the potential between atoms.

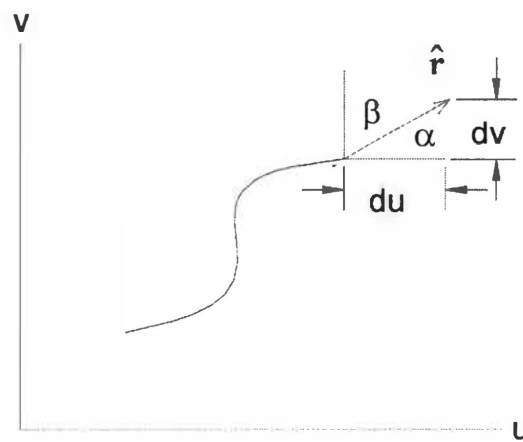


Figure 19: A sketch of the change of the position of the micro-cantilever's tip in the potential field by a distance of vector $\hat{r} = (\cos\alpha \hat{i} + \cos\beta \hat{j})$.

The force required to change the micro-cantilever tip's position by $\hat{r}$ is shown below to be the change in the potential energy along vector $\hat{r}$.

$$F_r = \frac{d\phi}{dr} \quad (18)$$

$$d\phi = F_r dr \quad (19)$$

Vector $\hat{r}$ can be converted to Cartesian coordinates using the following expression.

$$\hat{r} = (\cos\alpha \hat{i} + \cos\beta \hat{j}) \quad (20)$$

where $\hat{i}$ is the unit vector in the horizontal direction, and $\hat{j}$ is the unit vector in the vertical direction.

The force can also be written in terms of Cartesian coordinates as:

$$\frac{d\phi}{dr} = \frac{\partial\phi}{\partial u} \frac{du}{dr} + \frac{\partial\phi}{\partial v} \frac{dv}{dr} \quad (21)$$

$$F_r = \nabla\phi \cdot \hat{r} \quad (22)$$

where

$$\nabla = \frac{\partial}{\partial u} \hat{i} + \frac{\partial}{\partial v} \hat{j} \quad (23)$$

The components can be determined by multiplying Equation 22 by Equation 20.

$$F_u = \frac{d\phi}{du} = \left(\frac{\partial\phi}{\partial u} \hat{i} + \frac{\partial\phi}{\partial v} \hat{j} \right) \cdot (\cos\alpha \hat{i} + \cos\beta \hat{j}) \quad (24)$$

Given that $\hat{i}$ and $\hat{j}$ are unit vectors in the horizontal and vertical direction then $\cos\alpha \hat{i} = 1$ and that $\cos\beta \hat{j} = 0$, and Equation 24 reduces to the following.

$$\Rightarrow F_u = \frac{d\phi}{du} = \frac{\partial\phi}{\partial u} \quad (25)$$

$$\Rightarrow F_v = \frac{d\phi}{dv} = \frac{\partial\phi}{\partial v} \quad (26)$$

Looking at the change in the potential field along vector $\hat{r}$, which is tangent to contour line as seen in Figure 20; the potential energy along the contour lines is constant ($\phi(u, v) = \text{constant}$). Therefore, as shown by Equation 27, the change in the potential energy is equal to zero and therefore the change in the force is also equal to zero in the direction that is tangent to the lines of constant energy.

$$\frac{d\phi}{dr} = 0 \Rightarrow \nabla\phi \cdot \hat{r} = 0 \quad (27)$$

The change in the potential energy in a direction normal to the lines of constant energy as seen in Figure 21 is shown below in Cartesian coordinates.

$$F_n = \frac{\partial\phi}{\partial u} \cos\alpha + \frac{\partial\phi}{\partial v} \cos\beta \quad (28)$$

$$\Rightarrow F_n = |\nabla\phi| = \left[\left(\frac{\partial\phi}{\partial u} \right)^2 + \left(\frac{\partial\phi}{\partial v} \right)^2 \right]^{1/2} \quad (29)$$

Equation 29 is the force, or the directional derivatives of the potential energy field.

Atomic forces are therefore directionally dependent, with the magnitude being equal to the directional derivative of the potential energy. The derivative is broken into two components, the horizontal and the vertical. From these the forces in the horizontal and vertical direction can be determined. The atomic forces used to determine the motion of the micro-cantilever beam are based on these ideas.

Atomic Forces

The force between two atoms can be determined from the derivative of the potential energy. The derivative of Equation 8 gives the atomic force between atoms, where R is the distance between atoms.

$$\frac{\partial\phi(R)}{\partial R} = -\frac{12 B}{R^{13}} + \frac{6 A}{R^7} \quad (30)$$

Since Cartesian coordinates are being used in this study the potential energy is now

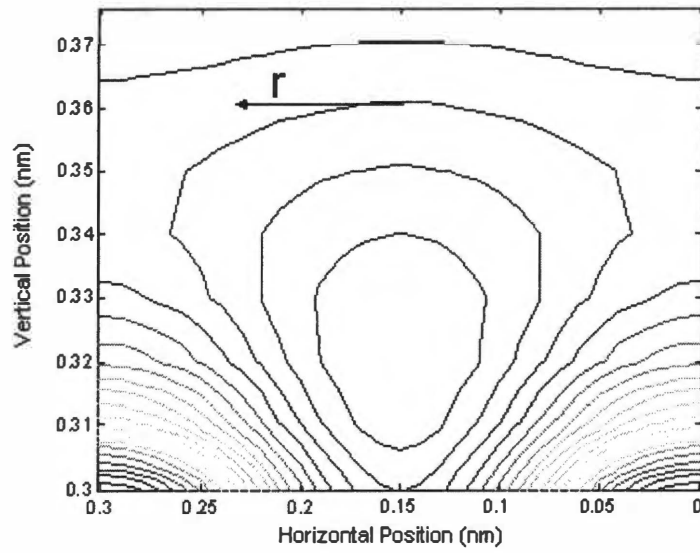


Figure 20: Lines of constant potential energy field, $\phi(u, v)$ of the atomic potential energy between two atoms with vector $\hat{r}$ tangent to lines of constant energy.

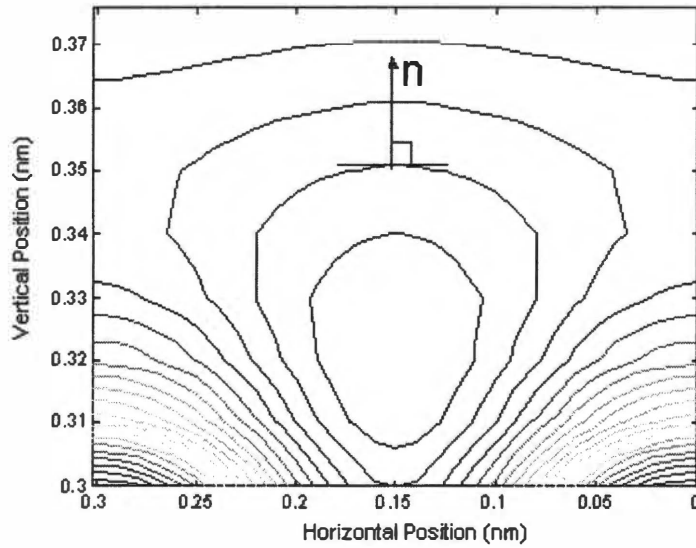


Figure 21: Lines of constant potential energy field, $\phi(u, v)$ of the atomic potential energy between two atoms with vector $\hat{n}$ normal to lines of constant energy.

dependent on two variables. The easiest way to determine the atomic force is to look at the derivatives in the horizontal, (u) and vertical, (v) directions. This is done by taking the derivative of the potential function as shown in Equation 13 with respect to u and v as seen below.

$$\frac{\partial \phi(u, v)}{\partial u} = -\frac{6(2u)B}{(u^2 + v^2)^7} + \frac{3(2u)A}{(u^2 + v^2)^4} \quad \text{Horizontal Force Component (31)}$$

$$\frac{\partial \phi(u, v)}{\partial v} = -\frac{6(2v)B}{(u^2 + v^2)^7} + \frac{3(2v)A}{(u^2 + v^2)^4} \quad \text{Vertical Force Component (32)}$$

The horizontal force component depends on both u and v. Since the horizontal force is currently of interest the force will be examined as a constant vertical offset as seen in Figure 22. The atomic spacing between atoms is typically on the order 0.3 nm to 0.5 nm or 3-5 Å. In this study an atomic spacing of 0.4 nm will be used for all calculations. Figure 22 shows the horizontal component of the force for a height equal to the atomic spacing, the force is periodic and appears to be sinusoidal. Note that the force is out of phase with the potential energy by 90°, which implies that the potential can be approximated as a cosine function. The force discussed here is based on static conditions. The tip has no dynamic motion.

Now we examine the vertical forces as a result of taking the derivative of Equation 13 with respect to y. The vertical force for an atom on top of another atom with no horizontal movement (x = 0) can be seen in Figure 23b. The static equilibrium position in Figure 23a is about 0.35 nm. Figure 24b shows the vertical force for a constant horizontal position (x value) midway between two atoms. The static equilibrium position in Figure 24a is about 0.322 nm. At both locations the trends have similar patterns, but different magnitudes. Both go to zero as the atom moves away from the surface, and they go to negative infinity as the atom moves closure to the surface. The negative force is a repulsive force trying to push the atoms away from each other.

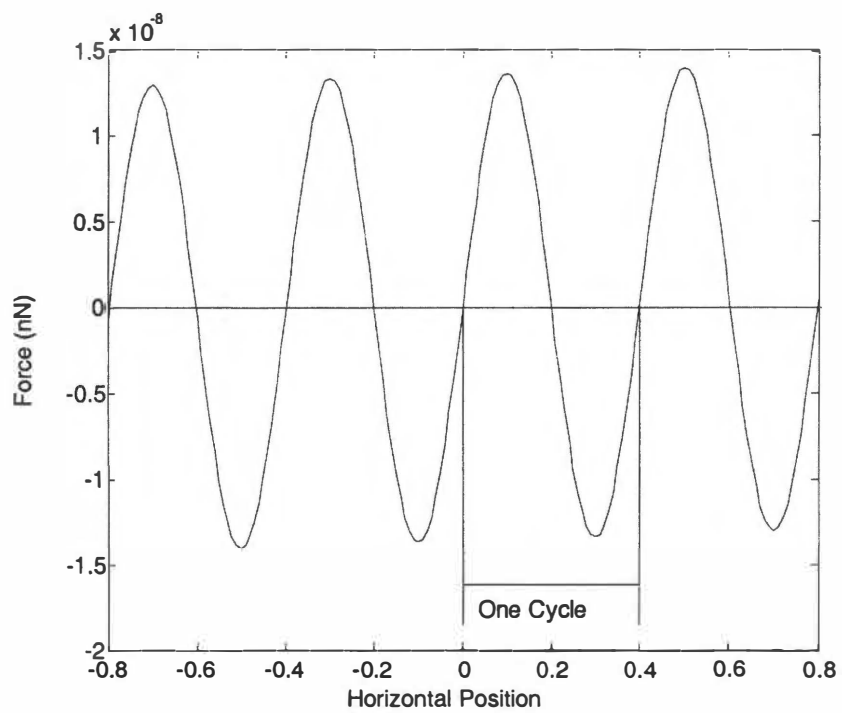


Figure 22: The horizontal force at a constant vertical offset Y_0 is 1 nm for an AS of 0.4 nm.

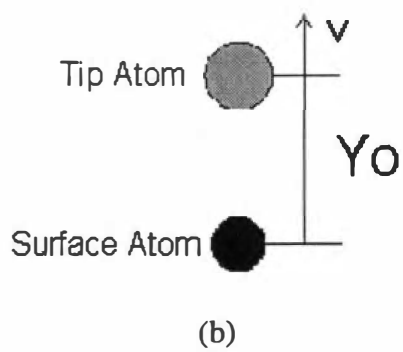
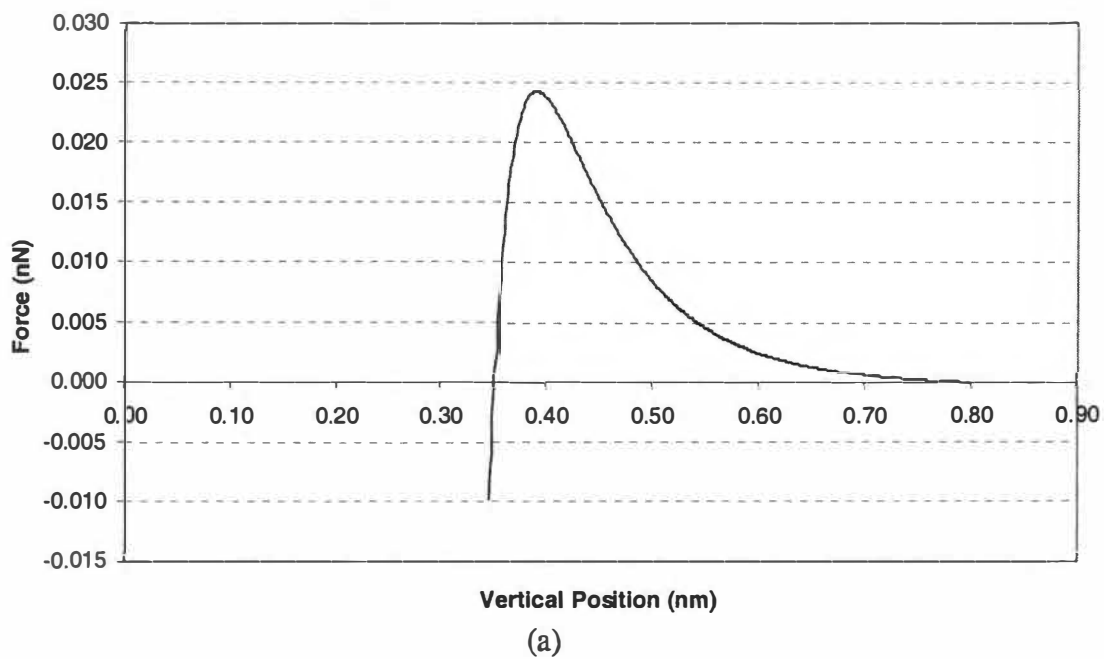


Figure 23: The vertical force (a) for an atom located directly over another atom as shown in sketch (b).

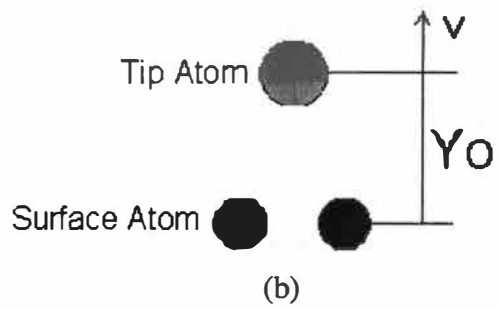
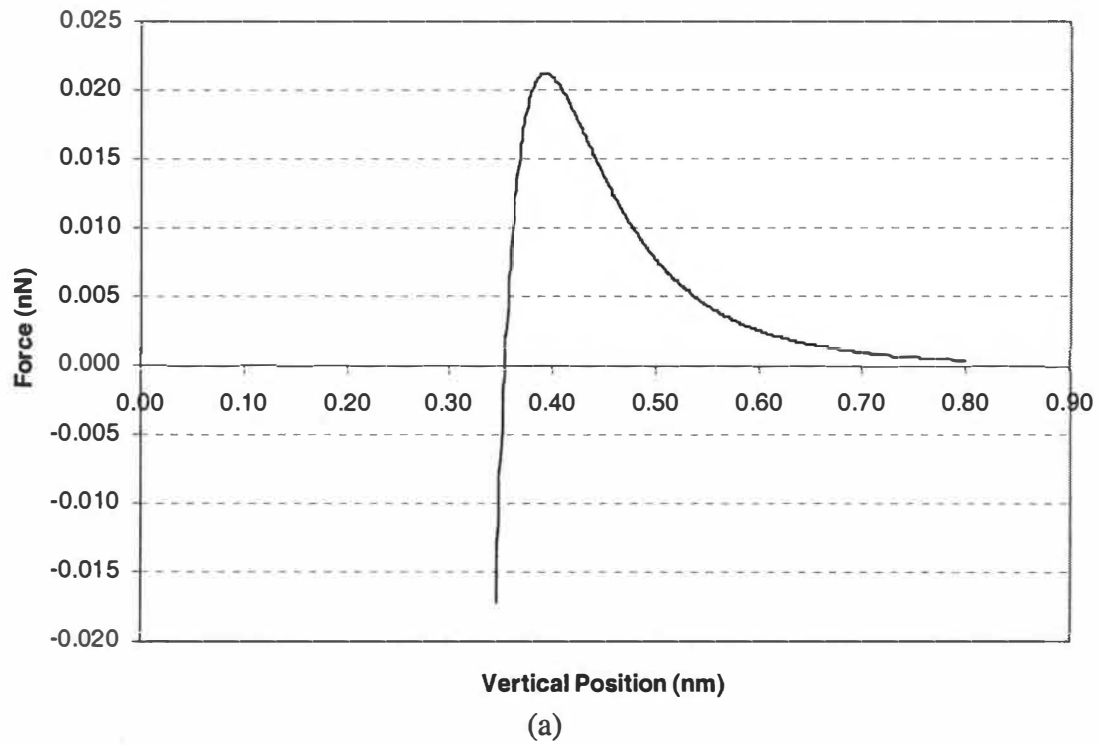


Figure 24: The vertical force (a) for an atom located between two atoms as shown in sketch (b).

Spring Force and Total Force

The micro-cantilever spring force is obtained by taking the derivative of the potential energy Equation 13 with respect to the horizontal and vertical directions, which are shown below.

$$\frac{\partial \phi_{spring}(u, v)}{\partial u} = (k_h)u \quad \text{Horizontal Spring Force} \quad (33)$$

$$\frac{\partial \phi_{spring}(x, y)}{\partial y} = (k_v)y \quad \text{Vertical Spring Force} \quad (34)$$

These forces are used to model the forces of the micro-cantilever beam due to its internal stiffness. The spring forces are simple linear relationships, which can be added directly to the horizontal or vertical atomic force to get the total horizontal or vertical force as shown below.

$$\frac{\partial \phi_{Total}(u, v)}{\partial u} = -\frac{6(2u)B}{(u^2 + v^2)^7} + \frac{3(2u)A}{(u^2 + v^2)^4} + (k_h)u \quad \text{(Total Horizontal Force)} \quad (35)$$

$$\frac{\partial \phi_{Total}(u, v)}{\partial v} = -\frac{6(2v)B}{(u^2 + v^2)^7} + \frac{3(2v)A}{(u^2 + v^2)^4} + (k_v)v \quad \text{(Total Vertical Force)} \quad (36)$$

Examples of the total horizontal and vertical force are shown below in Figures 25 and 26. In both figures the spring force is a dominant force when the spring constant value is large. The linear effect in Figure 25 is due to the cantilever spring.

Spring Constants

Atoms can be modeled as if they were attached to each other by tiny springs, and the springs can be modeled using Lennard-Jones. The equivalent spring can be modeled by determining the atomic spring constant between the atoms by taking the second derivative of Equation 8 with respect to R, the distance between atoms.

$$\frac{\partial^2 \phi(R)}{\partial R^2} = \frac{(13)(12)B}{R^{14}} - \frac{(7)(6)A}{R^8} \quad \text{(Atomic Spring Constant)} \quad (37)$$

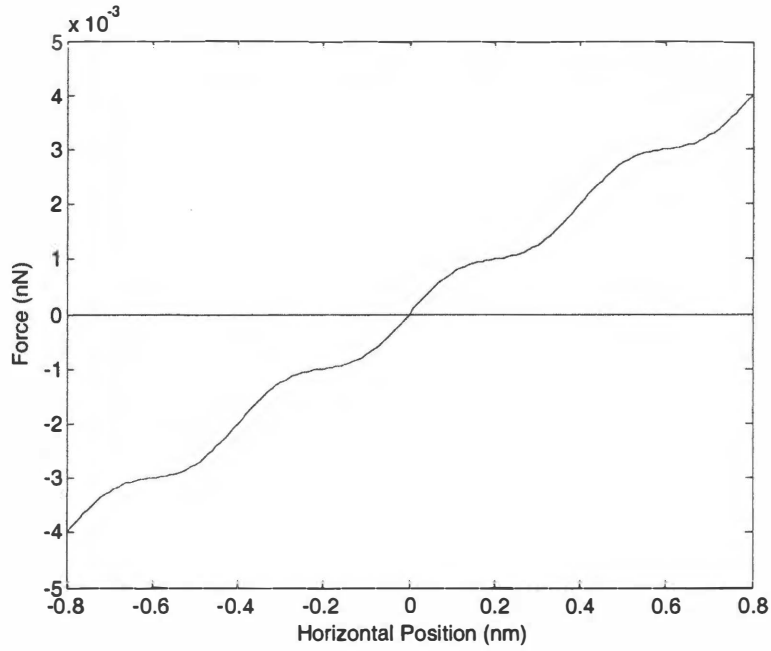


Figure 25: The total horizontal force required to move atom horizontally for a vertical offset $Y_0 = 0.5$ nm with the following parameters Spring Constant $k_h = 0.05$ nN/nm, and an atomic spacing (AS) = 0.4 nm.

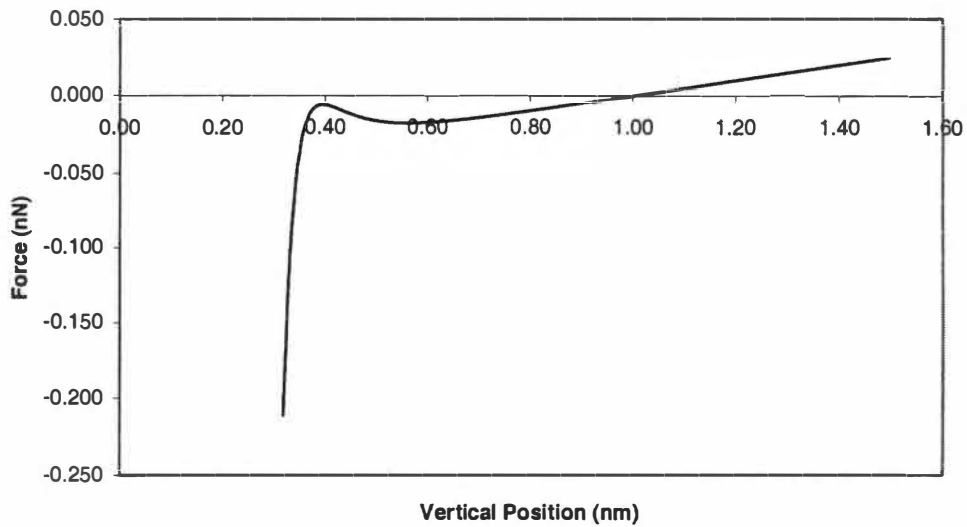


Figure 26: The total vertical force required to move atom vertically for an atom directly over another atom with the following parameters Spring Constant $k_v = 0.05$ nN/nm, and a vertical offset Y_0 of 1 nm.

The atomic spring constant defined by Equation 37 is the rate of change of the interactive forces and this changes with atomic spacing (R). A common use of this type of non-linear spring constant is the change in force is a function of the change in position, $\Delta F = k\Delta R$. For this study the spring constants need to be in Cartesian coordinates. This is done by taking the second derivative of Equation 13 with respect to both the horizontal (x) and the vertical (y) directions as shown below.

$$\frac{\partial^2 \phi(u, v)}{\partial u^2} = -\frac{6(2)B}{(u^2 + v^2)^7} + \frac{(7)(6)(4)u^2 B}{(u^2 + v^2)^8} + \frac{(4)(3)(4)u^2 A}{(u^2 + v^2)^5} + \frac{(3)(2)A}{(u^2 + v^2)^4} \quad (38)$$

$$\frac{\partial^2 \phi(u, v)}{\partial v^2} = -\frac{6(2)B}{(u^2 + v^2)^7} + \frac{(7)(6)(4)v^2 B}{(u^2 + v^2)^8} + \frac{(4)(3)(4)v^2 A}{(u^2 + v^2)^5} + \frac{(3)(2)A}{(u^2 + v^2)^4} \quad (39)$$

If the micro-cantilever's tip is at a vertical offset equal to the atomic spacing, the spring constants are periodic, and are approximately sinusoidal as seen in Figure 27. The pattern can be approximated by a negative cosine function.

The spring constant increase as the atoms move closer to the surface as seen in Figures 28a and 29a. Figure 28a shows the local vertical spring constant for an atom over atom shown in Figure 28b, and Figure 29a shows the local vertical spring constant when atoms is located midway between two atoms as shown in Figure 29b. The local spring constants are weaker in Figure 29a.

Total Spring Constants

The spring constants for the micro-cantilever beam are already known. Therefore the total equivalent spring constant for the system is the micro-cantilever beam spring constants added to the atomic spring constants as shown below.

$$\frac{\partial^2 \phi_{total}(u, v)}{\partial u^2} = -\frac{6(2)B}{(u^2 + v^2)^7} + \frac{(7)(6)(4)u^2 B}{(u^2 + v^2)^8} + \frac{(4)(3)(4)u^2 A}{(u^2 + v^2)^5} + \frac{(3)(2)A}{(u^2 + v^2)^4} + k_h \quad (40)$$

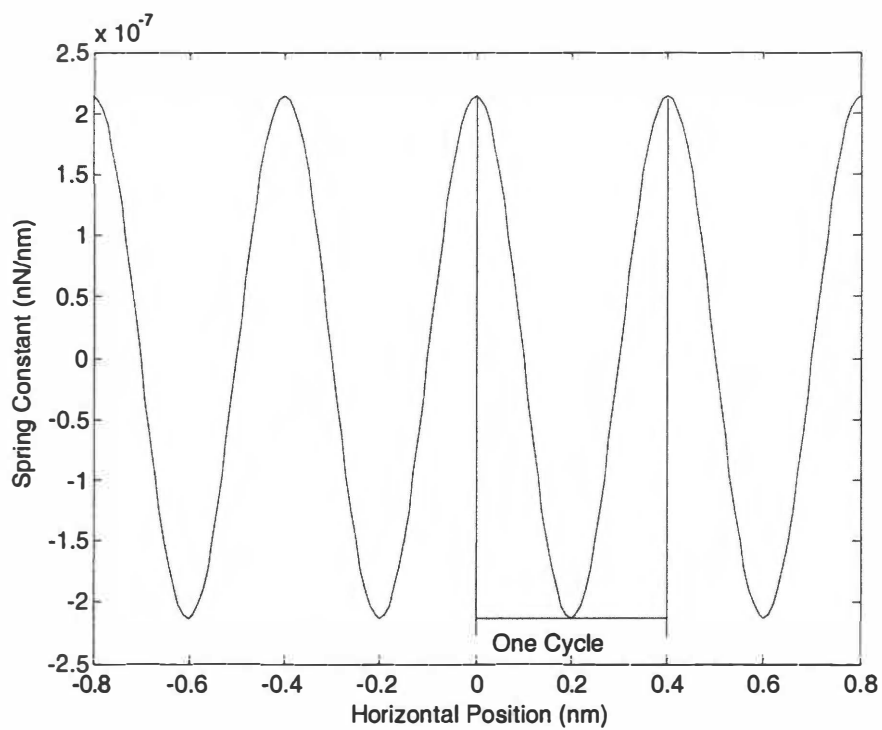
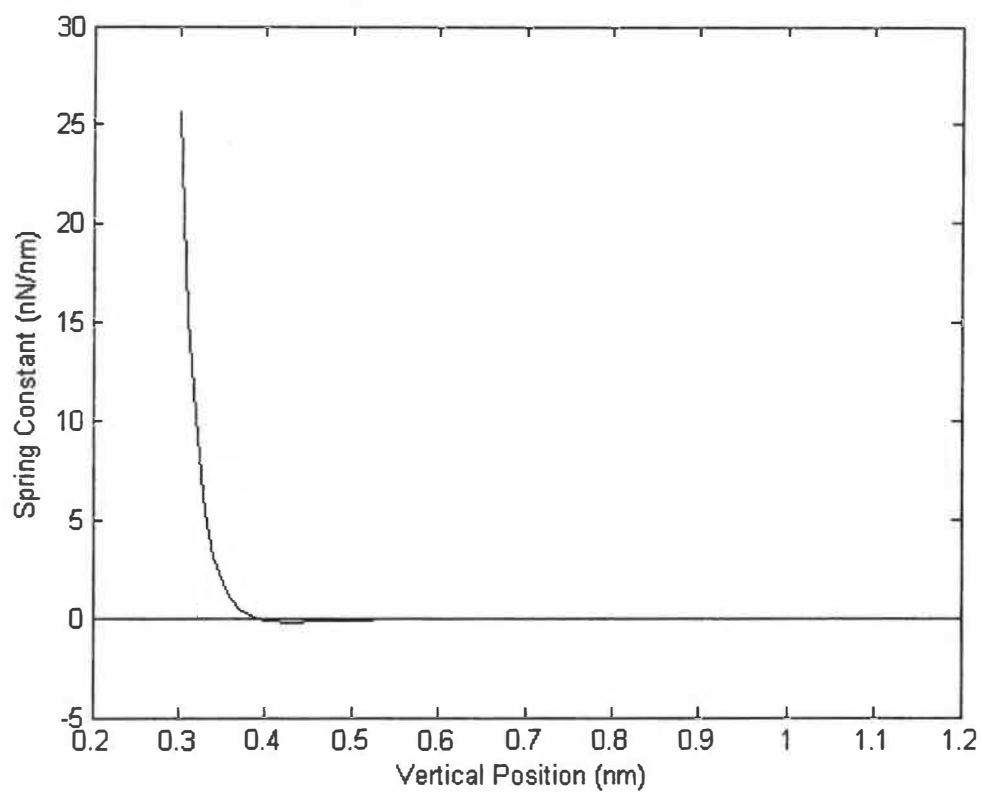
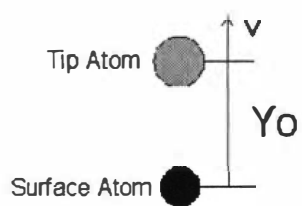


Figure 27: The horizontal spring constant at a constant vertical offset $Y_0 = 1$ nm for an AS of 0.4 nm.

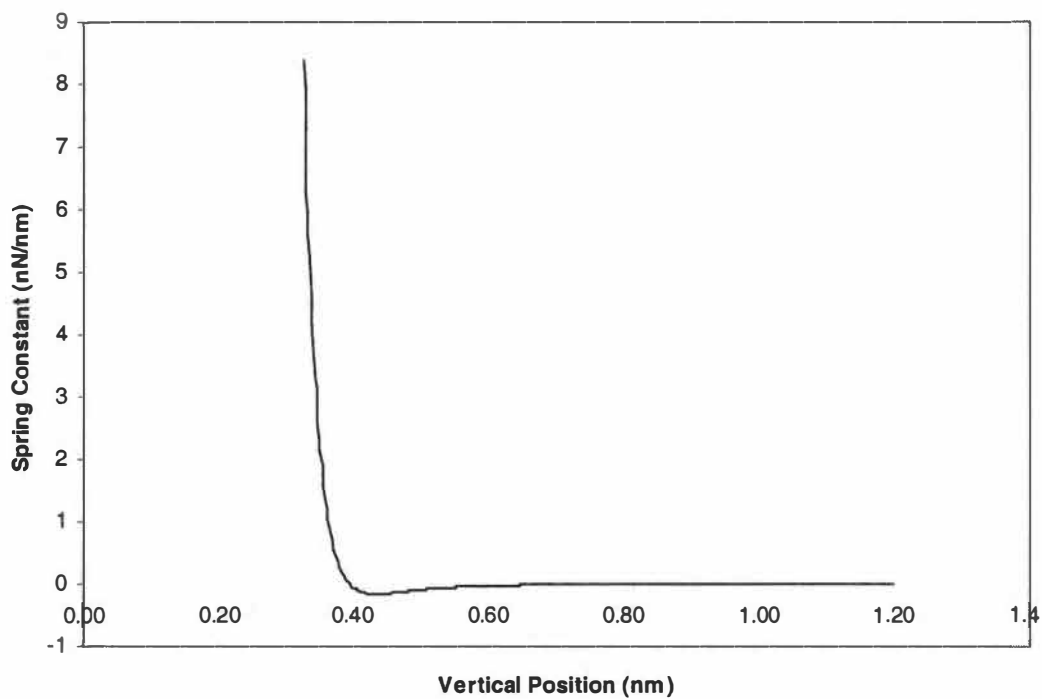


(a)

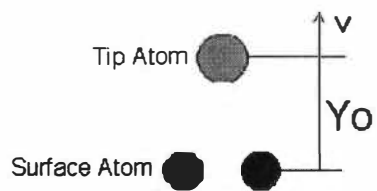


(b)

Figure 28: The local vertical spring constant (a) for an atom directly over another atom (b).



(a)



(b)

Figure 29: The local vertical spring constant (a) for an atom located between two atoms (b).

$$\frac{\partial^2 \phi_{total}(u, v)}{\partial v^2} = -\frac{6(2)B}{(u^2 + v^2)^7} + \frac{(7)(6)(4)v^2 B}{(u^2 + v^2)^8} + \frac{(4)(3)(4)v^2 A}{(u^2 + v^2)^5} + \frac{(3)(2)A}{(u^2 + v^2)^4} + k_v \quad (41)$$

Figures 29 and 30 show the total horizontal spring constants. At a height of 0.3 nm it is evident that the atomic spring constant is riding on the micro-cantilever's spring constant as shown in Figure 30. Figure 31 shows the atomic spring constant riding on the micro-cantilever's spring constant, which can be compared to the horizontal atomic spring constant in Figure 24 and 27. Figure 32 shows the total vertical spring constant, this is what one would expect to see. The local vertical atomic spring constant as seen in Figure 29a was added to the micro-cantilever's spring constant, which was 5 nN/nm.

In the next chapter the development of the physical model of the tip of the micro-cantilever beam will be discussed, and how the Lennard-Jones potential plays a part in predicting the dynamics.

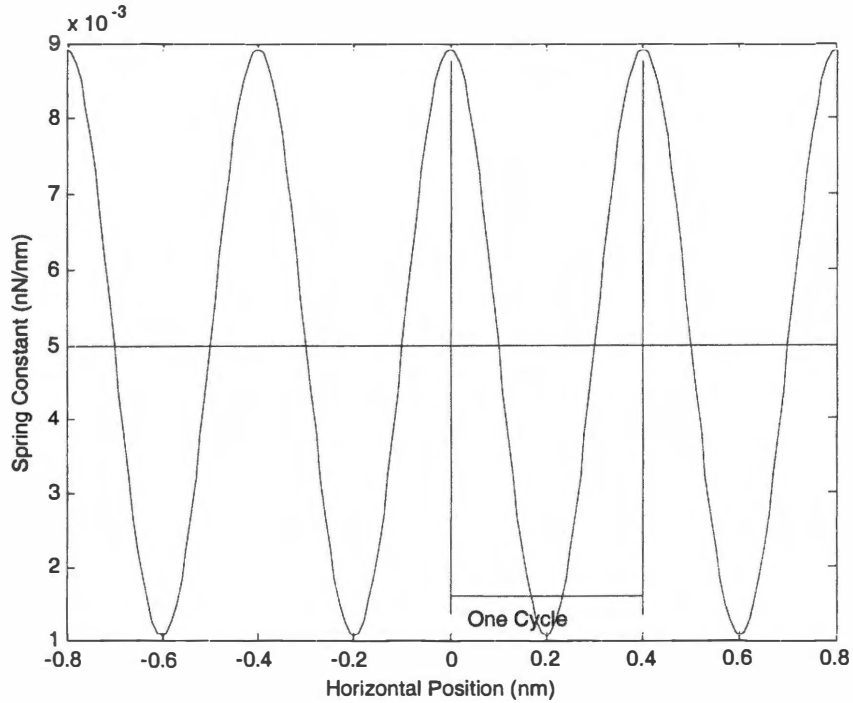


Figure 30: The total horizontal spring constant for $k_h=0.05$ nN/nm and a vertical offset Y_0 of 0.5 nm.

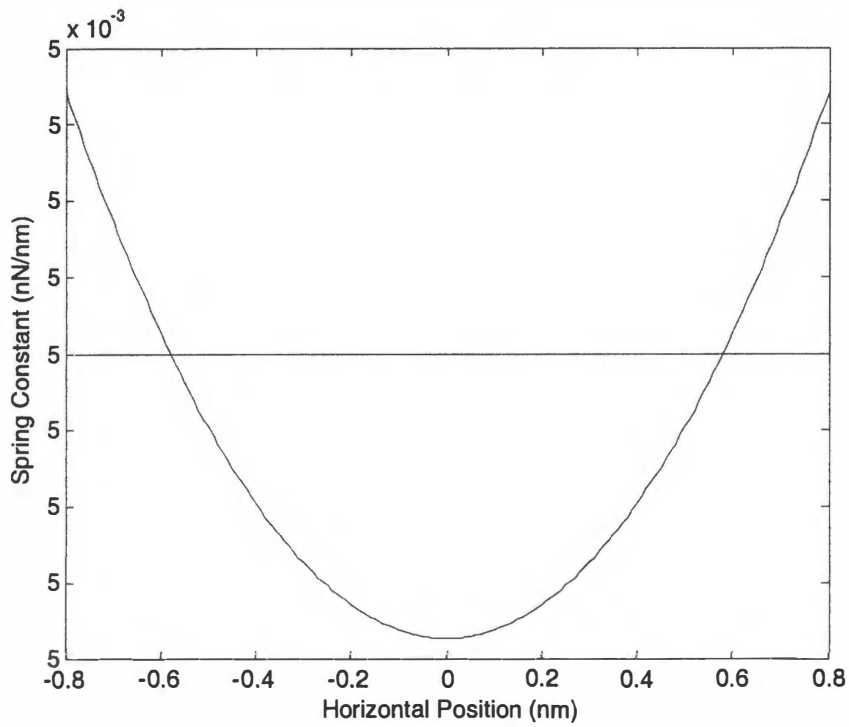


Figure 31: The total horizontal spring constant for $k_h=0.05$ nN/nm and a vertical offset Y_0 of 5.0 nm.

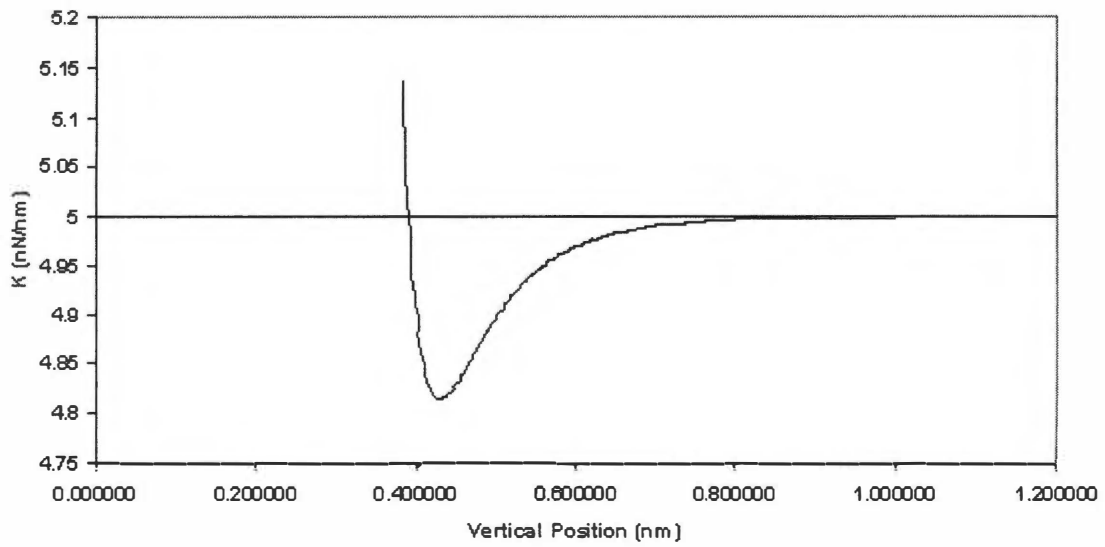


Figure 32: The total vertical spring constant for a cantilever stiffness of $k_v = 5$ nN/nm.

4 Simulating the Dynamics of the Micro-Cantilever Tip

Potential Field

In this section we will develop the differential equations of motion for the tip and explain how these non-linear differential equations are solved.

Potential energy field will drive the dynamics of the micro-cantilever tip. Figure 33 shows the potential field for a row of atoms, and the atom on the tip of the micro-cantilever beam. Since the potential energy field is so important, the Lennard-Jones potential relationship will be used to approximate the atomic potential field.

Sketch of System

The physical system for this study is defined in Figure 34. The sketch seen in Figure 34 is of the micro-cantilever, the tip of the micro-cantilever beam, and the atoms on the surface. The micro-cantilever/tip system is being modeled as a spring/mass system. This can be done because the equivalent spring constant for the cantilever beam and the natural frequency associated with that spring constant are known or have been determined experimentally. The equivalent mass can be calculated from the equivalent spring constant and the natural frequency.

The atom located at the origin of the (u, v) is the atom on the tip of the micro-cantilever. The black dots that run along the X axis are the atoms on the surface, and atomic spacing, AS is the distance between atoms or atomic spacing. The X_o and Y_o are coordinates used to locate the atoms on the surface relative to the atom on the micro-cantilevers tip. These coordinates (X_o, Y_o) do not change during any of the simulations.

Since the goal of this study is to examine how the dynamics of the tip of a micro-cantilever beam are driven by the atomic potential energy or atomic forces, it is necessary to simplify the model so that the atomic interactions are the only forces affecting the dynamics. To do this several assumptions were to be made as given below.

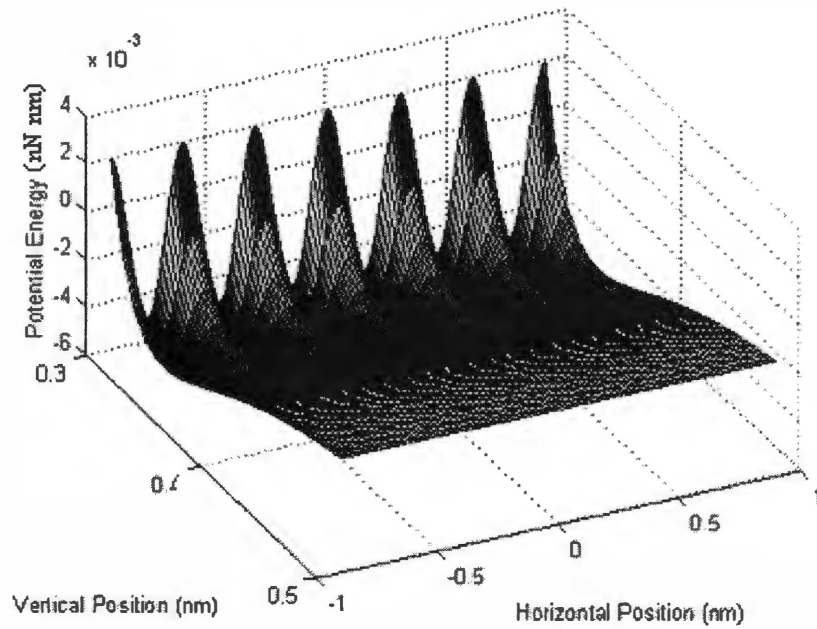


Figure 33: The atomic potential energy field $\phi(u, v)$ for an atomic spacing of 0.3 nm.

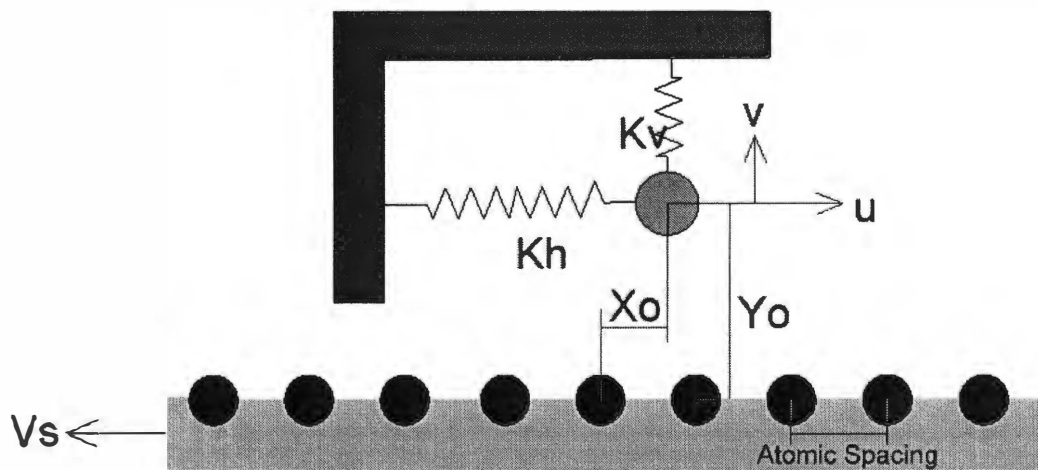


Figure 34: Sketch of micro-cantilever as a spring mass system above a row of atoms.

Assumptions

- Internal damping in the micro-cantilever can be neglected.
- No capillary forces or electrostatic forces are involved.
- Since the spring constant and natural frequency of the micro-cantilever beam are known then the system can be modeled as a spring mass system.
- The nearest atom on the tip interacts with the atoms on the surface.
- Assume an ideal surface one that is perfectly flat with no irregularities in the atoms' spacing.
- The Lennard-Jones potential is a good model for the interactive atomic forces.
- The Newmark Beta method is a good numerical non-linear solver for this problem.

Converting the Lennard-Jones Relationships

It is necessary to redefine the Lennard-Jones Potential Energy relationship and the cantilevers potential energy, from which the total force and total spring constant relationships are derived. This is done so that they are related to the system being modeled as seen in Figure 34. The relationships must take into account that there are now two coordinate systems, and that the row of atoms under the cantilever tip is now moving with some velocity, V_s (Scanning Velocity). By redefining the relationship for the Lennard-Jones potential energy the distance between atoms R can be shown as.

$$R = \sqrt{(X_0 + V_s * t + u)^2 + (Y_0 + v)^2} \quad (42)$$

Therefore the Lennard-Jones Potential becomes.

$$\phi(u, v, t) = \frac{B}{\left(\sqrt{(X_0 + V_s * t + u)^2 + (Y_0 + v)^2} \right)^{12}} - \frac{A}{\left(\sqrt{(X_0 + V_s * t + u)^2 + (Y_0 + v)^2} \right)^6} \quad (43)$$

The cantilever spring's potential energy is redefined so that the tip of micro-cantilever is in equilibrium when it is at the origin for the (u, v) coordinate system. Therefore the potential energy of the cantilever spring becomes:

$$\phi_{spring}(u, v) = \frac{1}{2}(kh)u^2 + \frac{1}{2}(kv)v^2 \quad (44)$$

The total force and total spring constant can be derived from the modified Lennard-Jones potential and the modified cantilever spring potential. The following are the modified total force relationships and the total spring constant relationships used in this study.

Total Horizontal Force

$$\begin{aligned} \frac{\partial \phi(u, v)}{\partial u} &= F_h \\ F_h &= -\frac{6(2X_o + 2V_s t + 2u)B}{((X_o + V_s t + u)^2 + (Y_o + v)^2)^7} + \frac{3(2X_o + 2V_s t + 2u)A}{((X_o + V_s t + u)^2 + (Y_o + v)^2)^4} + K_h u \end{aligned} \quad (45)$$

Total Vertical Force

$$\begin{aligned} \frac{\partial \phi(u, v)}{\partial v} &= F_v \\ F_v &= -\frac{6(2Y_o + 2v)B}{((X_o + V_s t + u)^2 + (Y_o + v)^2)^7} + \frac{3(2Y_o + 2v)A}{((X_o + V_s t + u)^2 + (Y_o + v)^2)^4} + K_v v \end{aligned} \quad (46)$$

Horizontal Atomic Spring Constant

$$\begin{aligned} \frac{\partial^2 \phi_{Total}(u, v)}{\partial u^2} &= -\frac{12B}{((X_o + V_s t + u)^2 + (Y_o + v)^2)^7} + \frac{42(2X_o + 2V_s t + 2u)^2 B}{((X_o + V_s t + u)^2 + (Y_o + v)^2)^8} \\ &\quad - \frac{12(2X_o + 2V_s t + 2u)^2 A}{((X_o + V_s t + u)^2 + (Y_o + v)^2)^5} + \frac{6A}{((X_o + V_s t + u)^2 + (Y_o + v)^2)^4} \end{aligned} \quad (47)$$

Vertical Atomic Spring Constant

$$\begin{aligned} \frac{\partial \phi^2_{Total}(u, v)}{\partial v^2} = & -\frac{12 B}{\left((X_0 + V_s t + u)^2 + (Y_0 + v)^2\right)^7} + \frac{42(2Y_0 + 2v)^2 B}{\left((X_0 + V_s t + u)^2 + (Y_0 + v)^2\right)^8} \\ & -\frac{12(2Y_0 + 2v)^2 A}{\left((X_0 + V_s t + u)^2 + (Y_0 + v)^2\right)^5} + \frac{6 A}{\left((X_0 + V_s t + u)^2 + (Y_0 + v)^2\right)^4} \end{aligned} \quad (48)$$

Equations 45 and 46 are the total external forces required to keep the tip of the micro-cantilever beam in equilibrium. These forces are the sum of all of the atomic forces and cantilever spring forces acting on the tip of the micro-cantilever beam. When the force is equal to zero, the micro-cantilever tip is in equilibrium.

To understand how the forces act on the tip of the micro-cantilever beam and their direction a free body diagram must be created. The free body of the tip of the micro-cantilever beam, as seen in Figure 35, simply shows all of the forces acting on the mass. The spring force of the micro-cantilever beam acts on the mass. This spring force is resolved into horizontal and vertical components as shown in Figure 35. The other forces acting on the mass are the atomic forces, which are a result of the interaction between the atom on the tip of the micro-cantilever and the atoms on the surface. It can be shown that only a finite number of atoms are needed in the calculation to establish the atomic forces between the tip and the surface. According to Equation 30, the atomic force is essentially zero for large values of R , and it becomes extremely high as R approaches zero. In order to approximate the atomic force acting on the cantilever tip an assumption is made that the number of atoms interacting with the tip is a small number. It is suggested that the minimum number of atoms to be included in the atomic force approximation is all atoms within a distance one or two atomic spaces on both side of the tip. However in this study the contribution of a small number of atoms on the surface will be included in the force calculations since the length of the surface is of a finite length less than 100-200 nm in length.

Free Body Diagram

The equations of motion can be determined from the free body diagram shown in Figure 35. The following set of differential equations, which describes the motion for a two-degree of freedom system.

$$m \ddot{u} = -\sum \frac{\partial \phi(u, v)}{\partial u} - k_h * u \quad (49)$$

$$m \ddot{v} = -\sum \frac{\partial \phi(u, v)}{\partial v} - K_v * v \quad (50)$$

It is important to note that the total force and spring constant are dependent on the location of the micro-cantilever's tip relative to the atoms on the surface. This is due to the Lennard-Jones approximation for the force and spring constant. The atomic force and spring constants are dependent on u and v as seen in Figure 34, and on time (t) due to the surface is moving under the tip. Therefore the total driving force and the total spring constant are non-linear, and should be solved using a numerical solver.

Newmark Beta Method as a Non-linear Solver

The Newmark Beta method was used to solve the non-linear equations of motion for the horizontal, vertical, and two-degree of freedom vibration problems. The Newmark Beta method is a step-by-step numerical method used to solve non-linear equations [37]. The Newmark Beta Method assumes that the acceleration is constant over a give time step. This method of solution is summarized below for the sake of completeness.

To account for non-linear damping and/or non-linear spring effects the equation of motion is written:

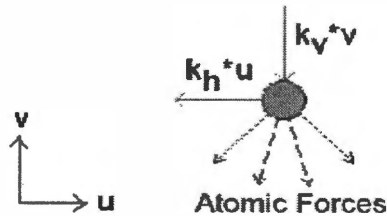


Figure 35: Sketch of the free body diagram of the mass for the spring mass system modeling the tip of the micro-cantilever beam.

$$m \ddot{u}_i + F_{di} + F_{si} = P_i \quad (51)$$

The acceleration is taken as the average acceleration between the time interval t to $t+1$.

$$\ddot{u}(\tau) = \frac{1}{2}(\ddot{u}_i + \ddot{u}_{i+1}) \quad (52)$$

Integrating Equation 52 twice gives

$$\dot{u}_{i+1} = \dot{u}_i + \left(\frac{\Delta t_i}{2} \right) (\ddot{u}_i + \ddot{u}_{i+1}) \quad (53)$$

$$u_{i+1} = u_i + \dot{u}_i \Delta t_i + \left(\frac{\Delta t_i^2}{2} \right) (\ddot{u}_i + \ddot{u}_{i+1}) \quad (54)$$

The equation of motion can be broken down into the following format, which because i and $i+1$ both satisfy the equation of motion.

$$m \Delta \ddot{u}_i + c_i \Delta \dot{u}_i + k_i \Delta u_i = \Delta p_i \quad (55)$$

Equation 53 and 54 can be used to determine the change in the acceleration $\Delta \ddot{u}_i$ and the velocity $\Delta \dot{u}_i$.

$$\Delta \ddot{u}_i = \left(\frac{4}{\Delta t_i^2} \right) (\Delta u_i - \dot{u}_i \Delta t_i) - 2 \ddot{u}_i \quad (56)$$

$$\Delta \dot{u}_i = \left(\frac{2}{\Delta t_i} \right) (\Delta u_i) - 2 \dot{u}_i \quad (57)$$

Equations 56 and 55 can be combined to give:

$$k_i^* \Delta u_i = \Delta p_i^* \quad (58)$$

Where

$$k_i^* = k_i + \left(\frac{2c}{\Delta t_i} \right) + \left(\frac{4m}{\Delta t_i^2} \right) \quad (59)$$

and

$$\Delta p_i^* = \Delta p_i + \left[\left(\frac{4m}{\Delta t_i} \right) + 2c \right] \dot{u}_i + 2m \ddot{u}_i \quad (60)$$

The change in the position, velocity, and acceleration can be determined by the following.

$$u_{i+1} = u_i + \Delta u_i \quad (61)$$

$$\dot{u}_{i+1} = \dot{u}_i + \Delta \dot{u}_i \quad (62)$$

$$\ddot{u}_{i+1} = \ddot{u}_i + \Delta \ddot{u}_i \quad (63)$$

Note that $\ddot{u}_i$ can also be determined from the equation of motion.

$$\ddot{u}_i = \left(\frac{1}{m} \right) \left(p_i - c \dot{u}_i - k u_i \right) \quad (64)$$

The step size for the constant time step should be $\Delta t_i \leq T/10$. T should be the smallest period of excitation or natural period. In our calculations “ c ”, the damping coefficient, was assumed to be zero. Also, $\Delta p_i = 0$ as the vibrations are driven by the non-linear springs of the atoms and the constant surface velocity, V_s .

Modeling the micro-cantilever tip as a single atom over a row of atoms allows for the two degree of freedom model of the tip to be simpler. The force derived from the Lennard-Jones potential makes it possible to determine the dynamics, and in the process the horizontal driving force acting on the micro-cantilever beam. Since the dynamics are based on a set of non-linear differential equations, it become necessary to use a non-linear solver like the Newmark Beta method to solve the equations of motion. In this case:

$$k_i = k + k_a \quad (65)$$

$$k_i = k + \frac{\partial^2 \phi}{\partial u^2} \quad (66)$$

where k_a is the non-linear atomic spring constant which varies with u and v .

We will study of three dynamic models. The first two are one-dimensional vibration models. The first is modeling the horizontal vibration with no vertical motion. The third model is a vertical vibration between two atoms with one attached to a spring. The last model to be studied is that of a two-dimensional vibration with two-degrees of freedom, which incorporates both horizontal and vertical motion.

5 Analysis of Dynamic Models

Three different dynamic simulations are analyzed in this study. First are the two basic models, which are the horizontal mode and the vertical mode. The two-degree of freedom vibration problem is the last model to be analyzed. It is the most important one because the dynamics of the micro-cantilever tip are determined, and the driving forces. A parameter study will be performed on the two degree of freedom model, but first the simpler cases must be examined. The following is a list of parameters used in the following studies.

$$\begin{aligned}f_v &= 20 \text{ kHz} & f_h &= 90 \text{ kHz} \\k_v &= 0.05 \text{ N/m (nN/nm)} & k_h &= 1.0125 \text{ N/m (nN/nm)} \\mass_{\text{effective}} &= 3.16629\text{E}^{-12} \text{ Kg}\end{aligned}$$

Horizontal Vibration (One-Degree of Freedom)

The tip of the micro-cantilever beam is not allowed to have any vertical displacement while the surface moves under the cantilever's tip. Also, there is no damping. A sketch of the system can be seen in Figure 36a. The Y_0 variable is constant and is only used in calculating the Lennard-Jones forces. In this dynamic model, the single atom that interacts with the surface is located on the cantilever tip. The spring k_h represents the horizontal flexibility of the micro-cantilever. The sample surface, which includes the row of atoms moves to the left with a constant surface velocity, V_s . The frame supporting the spring is fixed. The free body diagram of the single atom including the forces is given in Figure 36 b.

The equations of motion for the horizontal vibration model are the following:

$$m \ddot{u} = -k_h * u - (F_{LJ})_u \quad (67)$$

$$m \ddot{u} + k_h * u = -(F_{LJ})_u \quad (68)$$

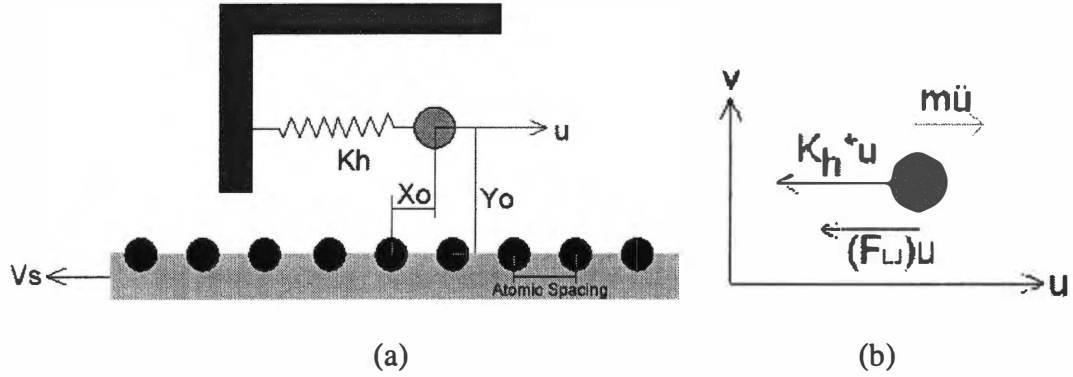


Figure 36: Sketch of Horizontal Dynamic Model (a) and Free Body Diagram (b).

Note that

$$(F_{LJ})_u = \frac{d\phi}{du} \quad (69)$$

where $\phi(u, v, t)$ is the total atomic potential field between the single atom and the sample surface atoms. The potential function, ϕ varies with time because the sample surface atoms are assumed to move to the left with velocity V_s . In this particular case $\phi = \phi(u, t)$, since Y_0 is constant and “ v ” is equal to zero.

In the equation of motion “ m ” is the equivalent mass of the micro-cantilever beam, and k_h is the horizontal spring constant of the micro-cantilever beam. The solutions to the equations of motion are obtained by using the Newmark Beta method to solve the non-linear equation of motion. The horizontal driving force is the horizontal component of the Lennard-Jones force, which is the driving force behind the vibration.

Horizontal Dynamic Solution

The Figures 37 - 40 show the horizontal motion of the micro-cantilever tip as a function of time and the horizontal force or driving force. Figure 37 shows that at low surface velocities the motion of the tip is sinusoidal, and that the horizontal force or driving force is the same as the static force seen in Figure 22. The magnitude of the displacement is small due to the fact that the horizontal forces acting on the tip are

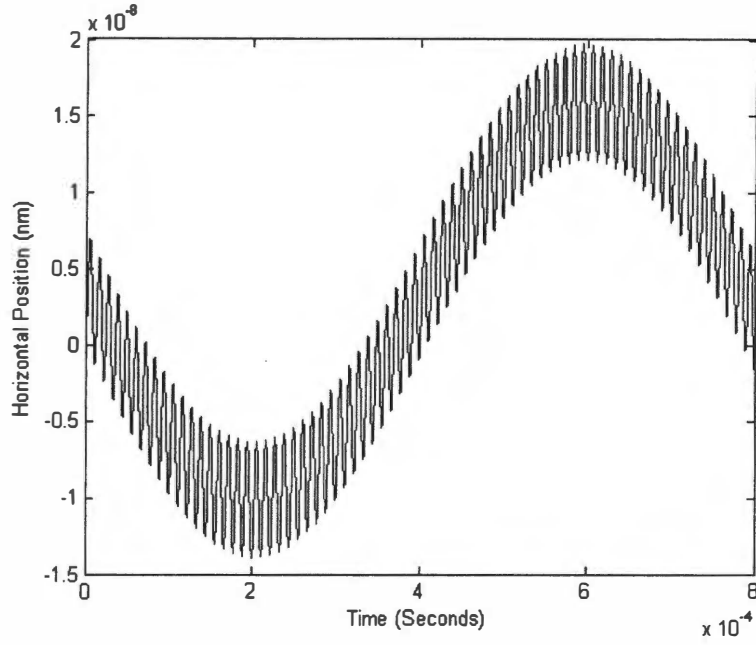


Figure 37: The horizontal motion of the micro-cantilever tip based on: A vertical offset $Y_o = 1.0$ nm, horizontal spring constant $k_h = 1.0125$ nN/nm, horizontal natural frequency of 90 kHz, surface velocity of 500 nm/s, $AS = 0.4$ nm.

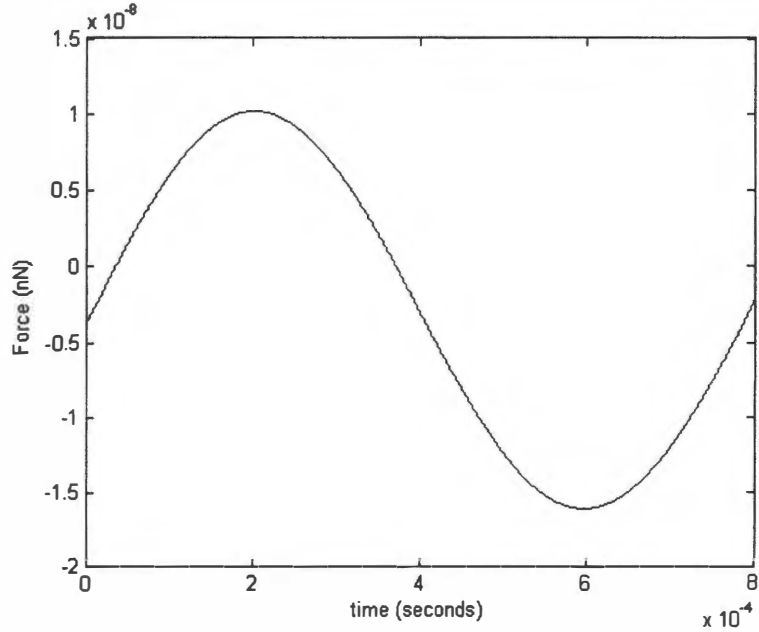


Figure 38: The horizontal force or driving force felt by the micro-cantilever tip based on: A vertical offset $Y_o = 1.0$ nm, horizontal spring constant $k_h = 1.0125$ nN/nm, horizontal natural frequency of 90 kHz, surface velocity of 500 nm/s., $AS = 0.4$ nm.

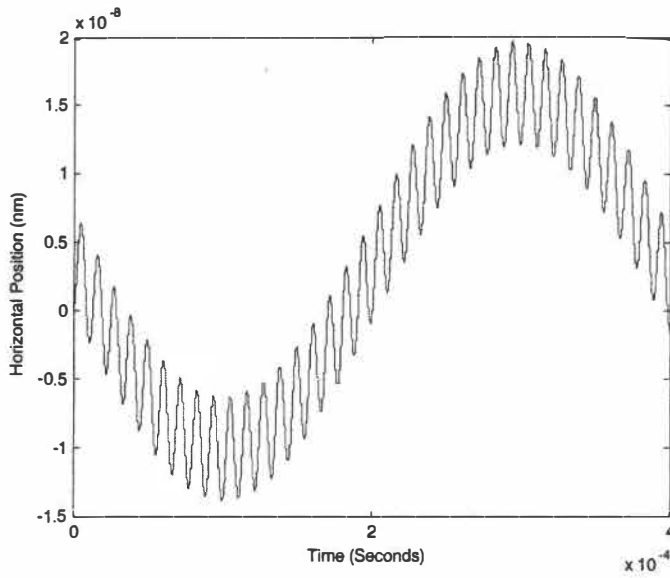


Figure 39: The horizontal position of the micro-cantilever tip based on: A vertical offset $Y_0 = 1.0$ nm, horizontal spring constant $k_h = 1.0125$ nN/nm, horizontal natural frequency of 90 kHz, surface velocity of 1000 nm/s, $AS = 0.4$ nm.

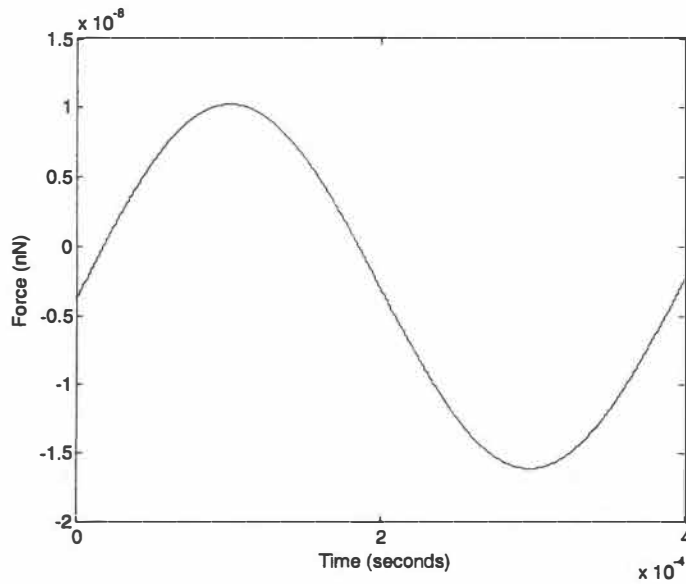


Figure 40: The horizontal force or driving force felt by the micro-cantilever tip based on: A vertical offset $Y_0 = 1.0$ nm, horizontal spring constant $k_h = 1.0125$ nN/nm, horizontal natural frequency of 90 kHz, surface velocity of 1000 nm/s, $AS = 0.4$ nm.

weaker than the vertical forces, and that the Lennard-Jones forces are based on $1/R^n$. This means that as R increases the force will decrease in magnitude. Note that the period of the vibration is equal to the atomic spacing. The oscillatory pattern seen riding the vibration is due to the horizontal component of the natural frequency of the micro-cantilever, which is f_h . Figure 39 shows that increasing the surface velocities results in the period of the vibration to change as shown in the time scale between the vibration plots.

Vertical Vibration (One-Degree of Freedom)

The next model being studied is the vertical vibration of the tip of the micro-cantilever beam as it is released from rest over another atom as seen in Figure 41a. In this model the goal is to view the vertical motion of the micro-cantilever specifically around the equilibrium points for the atomic potential and cantilever spring's potential independent of the horizontal motion of the single atom. Note that there is no horizontal motion in the tip, and the surface atom is fixed.

Therefore u and V_s in the Lennard-Jones equations are equal to zero, and the Lennard-Jones equations are now only dependent on " v ". The free body diagram for this case is shown in Figure 41b. Note that Y_0 is taken as the position of zero vertical spring force (ignoring the weight of the atom). Also the origin for determining motion v is located at Y_0 distance from the surface. The equations of motion for the vertical free vibration (no surface velocity, V_s) of the single atom (from the free body diagram) is

$$m \ddot{v} = -k_v * v - (F_{LJ})_v \quad (70)$$

$$m \ddot{v} + k_v * v = -(F_{LJ})_v \quad (71)$$

where

$$(F_{LJ})_v = \frac{d\phi}{dv} \quad (72)$$

and $\phi = \phi(v)$

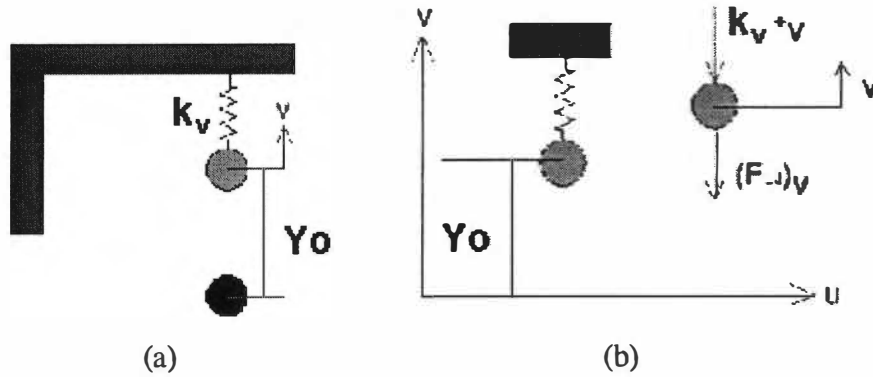


Figure 41: Sketch of Vertical Dynamic model (a) and Free Body Diagram (b).

In the equations of motion “ m ” is the equivalent mass of the micro-cantilever beam, and k_v is the micro-cantilever vertical spring constant. Y_0 is the offset distance of the micro-cantilever tip corresponding to zero spring loads. The Newmark Beta method is used to solve the above equations of motion. However there is an initial value given to “ v ” in the model, which defines the initial starting point for the vibration.

Figures 44-46 show the vertical free vibration and the vertical dynamic force felt by the tip of the micro-cantilever. Figure 42 is the total vertical potential energy for this dynamic model. Figure 43 shows the dynamic vertical force relative to the tip’s position. Figure 44 shows the tip vibrating back and forth between the spring and the atomic springs when it is started at $v_0 = 0.48$ nm, which vibrates between points of equal potential energy as seen in Figure 42. Figure 45 show a free vibration starting at $v_0 = -0.35$ nm which vibrates about the atomic equilibrium as seen in Figure 42. Figure 46 the free vibration starting at $v_0 = 0.05$ nm, which is a spring vibration about the spring’s equilibrium point. An increase spring constant or changing the vertical offset Y_0 can reduce the potential curve so that there is only one equilibrium point.

Two-Dimensional Vibration (Two-Degrees of Freedom)

The final model being studied is the two-dimensional or two degree of freedom model as seen in Figure 47a with a surface moving underneath the tip of the micro-cantilever at a surface speed of V_s in nm/s. The tip is allowed to move only in the vertical and horizontal direction there is no motion in the z direction.

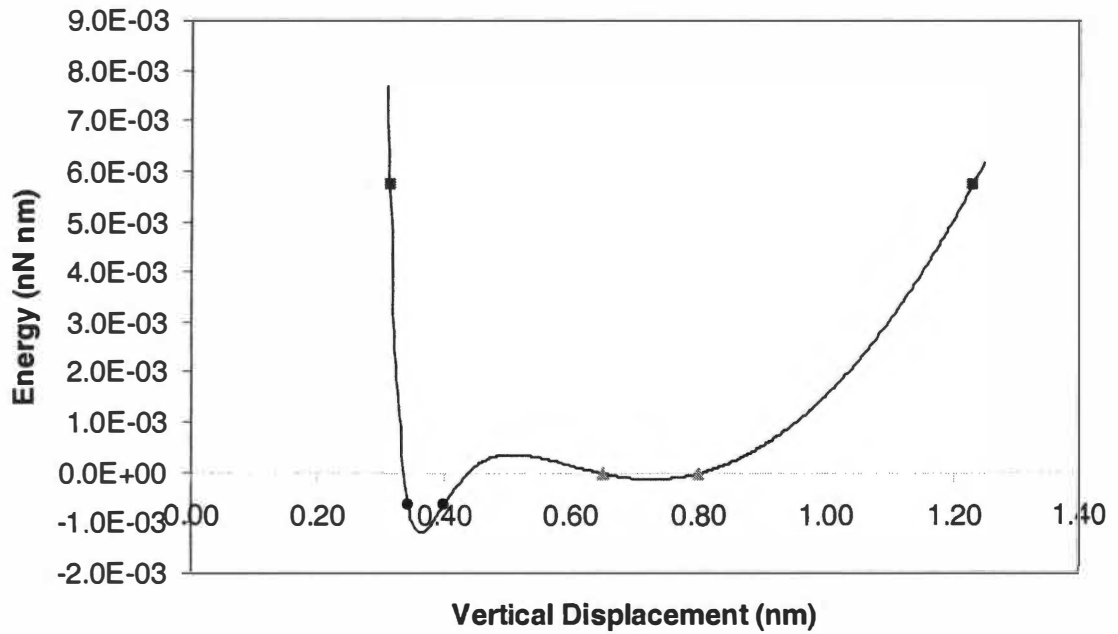


Figure 42: The total vertical potential energy for $Y_o = 0.75$ nm, spring constant $k_v = 0.05$ nN/nm.

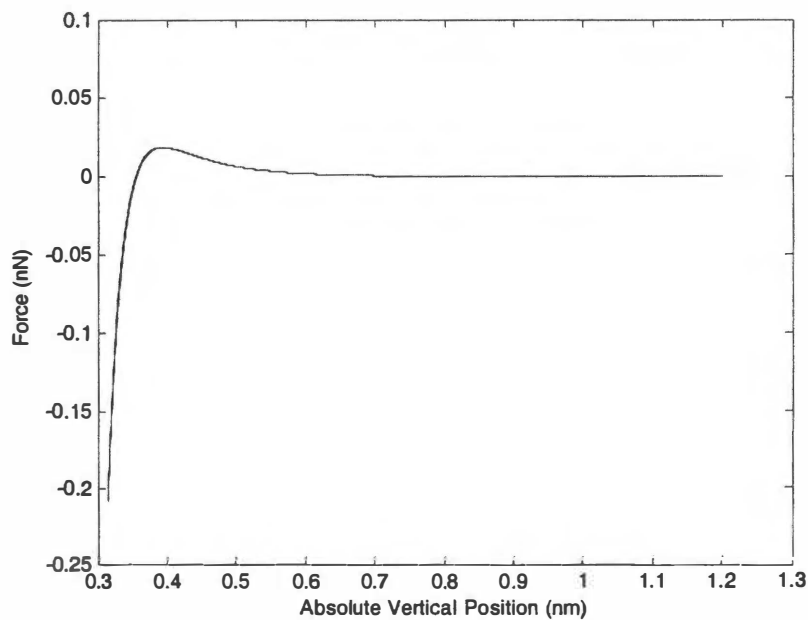


Figure 43: The vertical dynamic force is based on the following conditions Initial vertical position $v_o = 0.48$ nm, $Y_o = 0.75$ nm, spring constant $k_v = 0.05$ nN/nm, a natural frequency of 20 kHz.

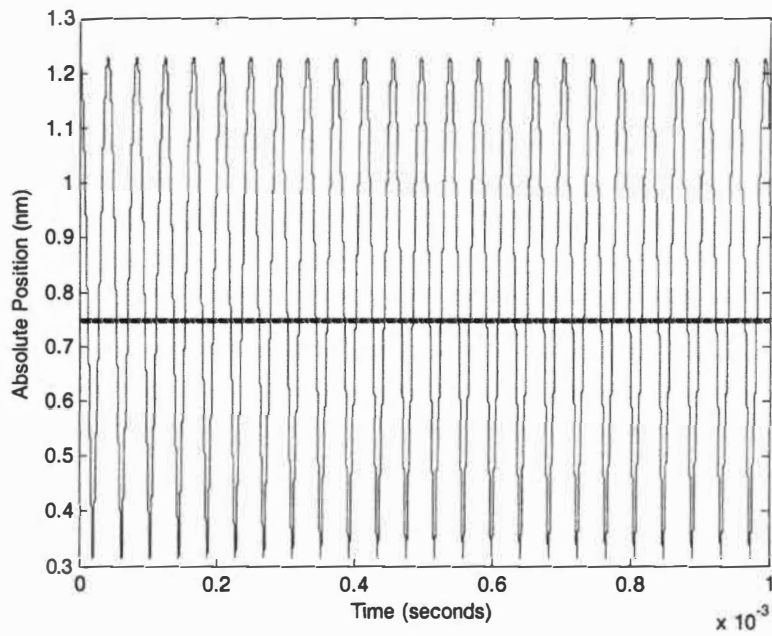


Figure 44: The absolute motion of the tip based on the following conditions. Initial vertical position $v_0 = 0.48$ nm, $Y_0 = 0.75$ nm, spring constant $k_v = 0.05$ nN/nm, a natural frequency of 20 kHz.

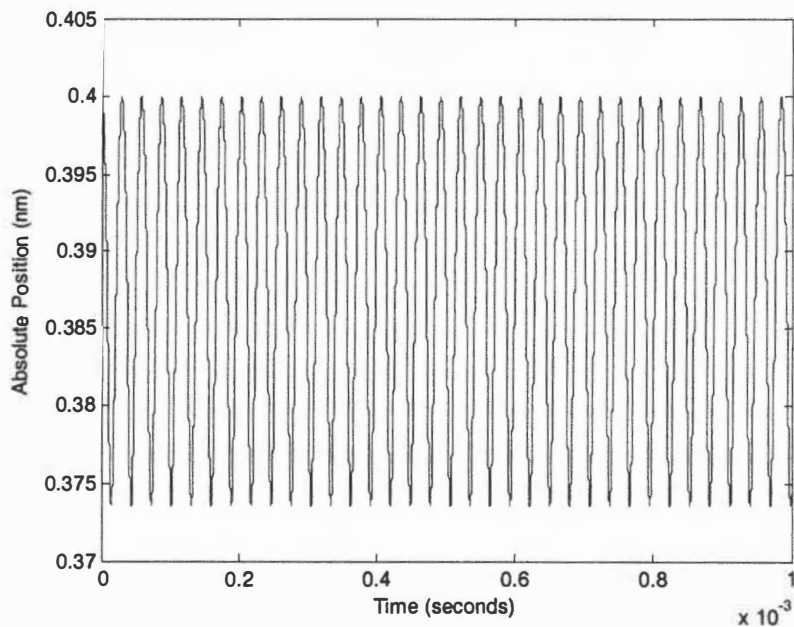


Figure 45: The absolute motion of the tip based on the following conditions. Initial vertical position $v_0 = -0.35$ nm, $Y_0 = 0.75$ nm, spring constant $k_v = 0.05$ nN/nm, a natural frequency of 20 kHz.

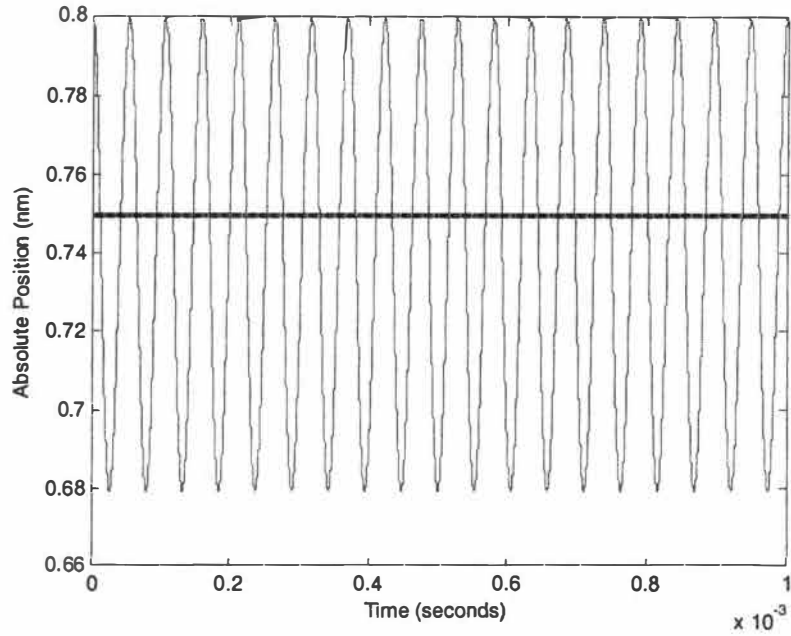


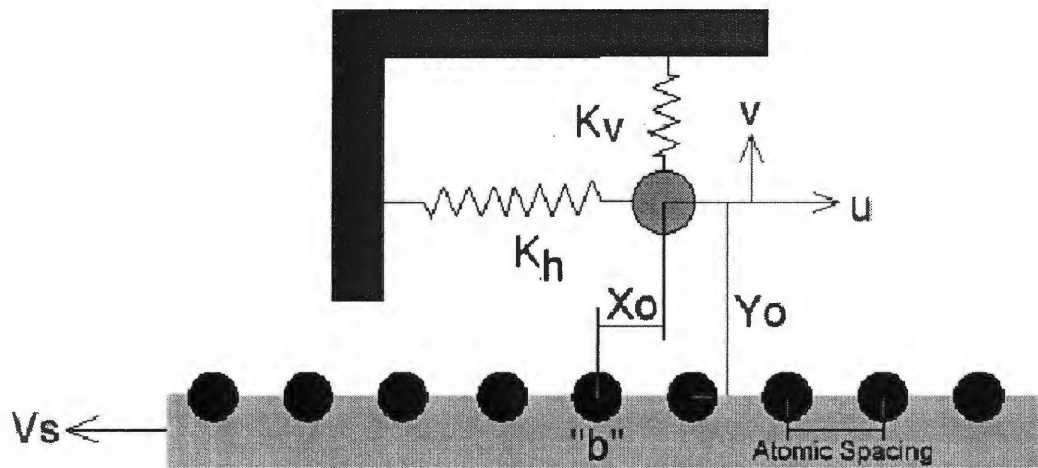
Figure 46: The Absolute tip position above is based on the following conditions. Initial vertical position $v_0 = 0.05$ nm, $Y_0 = 0.75$ nm, spring constant $k_v = 0.05$ nN/nm, a natural frequency of 20 kHz.

The Two-Dimensional motion of single atom is measure from u, v whose origin is fixed in space and located from the point of zero load in both the horizontal and vertical springs. Also, at time $t = 0$ seconds, the surface atom “b” is directly below the origin of the u, v axis.

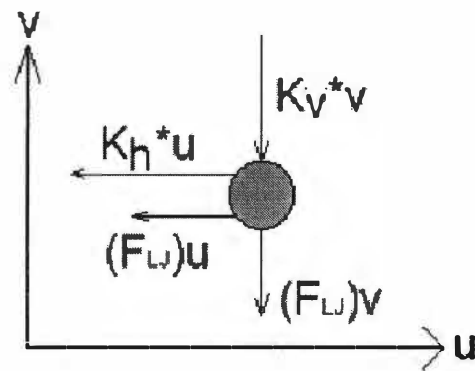
Recall that the total atomic potential is in terms of u, v , and V_s is

$$\varphi(u, v, t) = \frac{B}{\left(\sqrt{(X_0 + V_s * t + u)^2 + (Y_0 + v)^2} \right)^{12}} - \frac{A}{\left(\sqrt{(X_0 + V_s * t + u)^2 + (Y_0 + v)^2} \right)^6} \quad (73)$$

The differential equations of motion for the single atom are developed from the free body diagram in Figure 47b. The differential equation for the horizontal component u of motion is



(a)



(b)

Figure 47: Sketch of Two-Dimensional Dynamic model (a) and Two-Dimensional Free Body Diagram (b).

$$m \ddot{u} = -k_h * u - (F_{LJ})_u \quad (74)$$

or

$$m \ddot{u} + k_h * u = -(F_{LJ})_u \quad (75)$$

and for the vertical component v the differential equation of motion is

$$m \ddot{v} = -k_v * v - (F_{LJ})_v \quad (76)$$

or

$$m \ddot{v} + k_v * v = -(F_{LJ})_v \quad (77)$$

where

$$(F_{LJ})_u = \frac{d\phi}{du} = \frac{\partial\phi}{\partial u} \quad (78)$$

$$(F_{LJ})_v = \frac{d\phi}{dv} = \frac{\partial\phi}{\partial v} \quad (79)$$

In the equations of motion “ m ” is the equivalent mass of the micro-cantilever beam, k_h is the micro-cantilever horizontal spring constant, k_v is the micro-cantilever vertical spring constant. The origin of (u, v) is the no-load position of the micro-cantilever tip.

This is done so the spring equilibrium point is the point where there is no load on the micro-cantilever spring. The Newmark Beta method is used to solve the above non-linear equations of motion.

The following figures show the motion of the cantilever’s tip, and the total force that the tip feels. All the following figure are based on the cantilever beam having a vertical natural frequency of 20 kHz and a vertical spring constant, k_v of 0.05 nN/nm, and the horizontal natural frequency of 90 kHz and a corresponding horizontal spring constant, k_h of 1.0125 nN/nm. The cantilever has an initial offset above the surface Y_0 of 0.7 nm above the surface; the surface velocity is 500 nm/s, and an atomic spacing of 0.4 nm.

Figure 48 shows the vertical potential energy for the following dynamic plots. Figures 49-52 show the two-degree of freedom motion of the micro-cantilever tip, the horizontal motion, vertical motion, and the driving force felt by the tip.

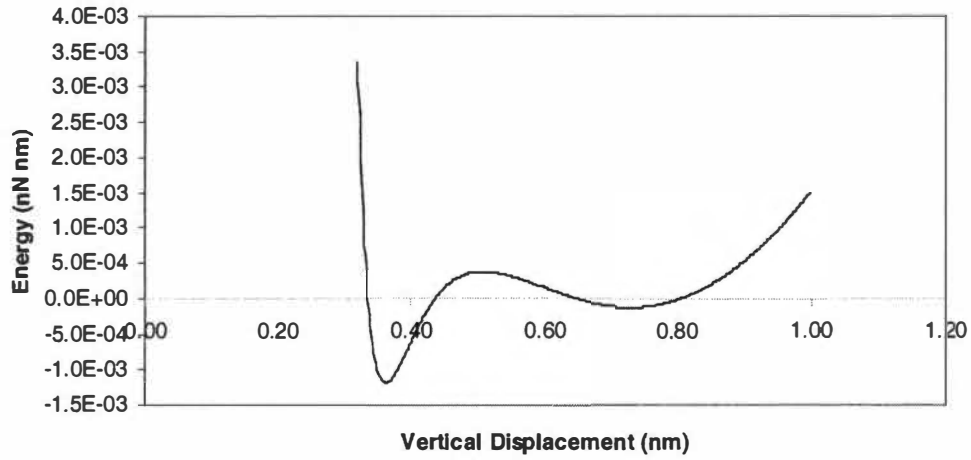


Figure 48: Vertical potential energy for a $k_v = 0.05$ nN/nm and a $Y_o = 0.75$ nm.

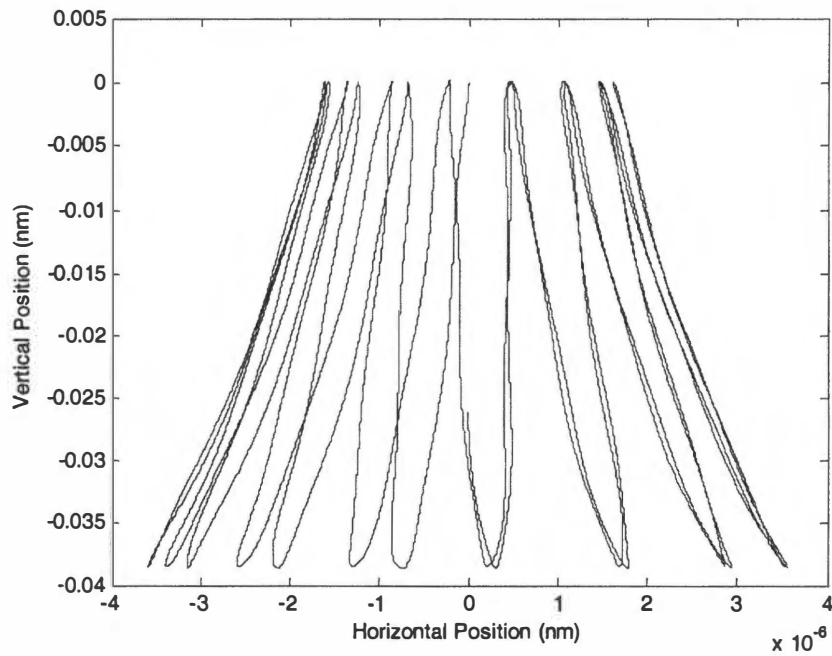


Figure 49: Two-Dimensional spatial motion of the tip of the micro-cantilever beam is based on the following $k_v = 0.5$ nN/nm, $k_h = 1.0125$ nN/nm, $AS = 0.4$ nm, and $V_s = 500$ nm/s, $Y_o = 0.75$ nm.

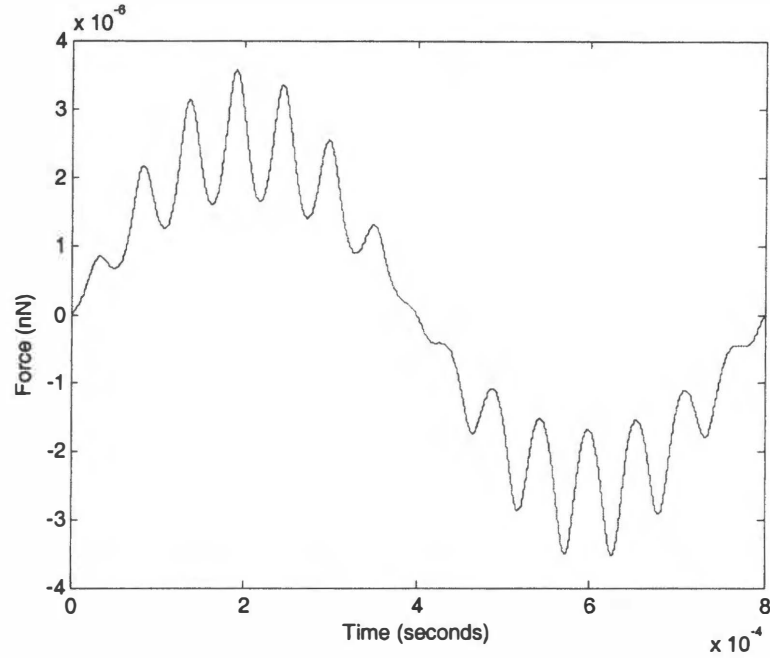


Figure 50: Horizontal Force or Driving Force the tip of the micro-cantilever feels is based on the following $k_v = 0.5 \text{ nN/nm}$, $k_h = 1.0125 \text{ nN/nm}$, $AS = 0.4 \text{ nm}$, and $V_s = 500 \text{ nm/s}$, $Y_o = 0.75 \text{ nm}$.

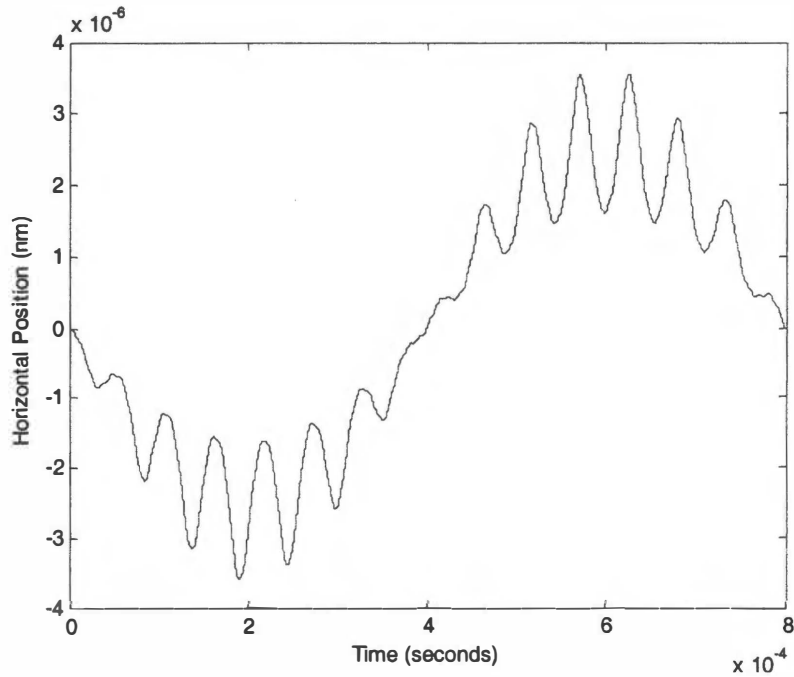


Figure 51: The horizontal motion of the micro-cantilever tip is based on the following $k_v = 0.5 \text{ nN/nm}$, $k_h = 1.0125 \text{ nN/nm}$, $AS = 0.4 \text{ nm}$, and $V_s = 500 \text{ nm/s}$, $Y_o = 0.75 \text{ nm}$.

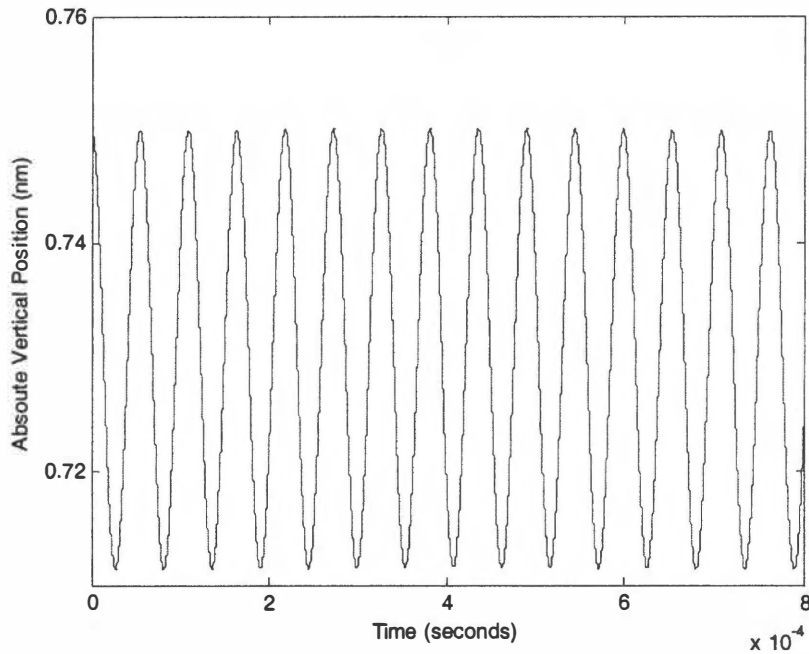


Figure 52: The absolute vertical motion of the micro-cantilever tip is based on the following $k_v = 0.5 \text{ nN/nm}$, $k_h = 1.0125 \text{ nN/nm}$, $AS = 0.4 \text{ nm}$, and $V_s = 500 \text{ nm/s}$, $Y_o = 0.75 \text{ nm}$.

Figure 49 shows the two-dimensional motion of the micro-cantilever tip. Figure 50 shows the force that the tip feels over a period of time, and Figures 51 and 52 shows the horizontal and vertical motion of the micro-cantilever tip over the same time interval. One thing to note is that the horizontal motion of the tip is much smaller than the vertical motion so the focus of the parameter study will be on just the vertical motion of the tip and the horizontal driving force the tip feels.

A parameter study will be done for the two degree of freedom problem. The variable that are of importance are the vertical offset Y_o and the surface velocity V_s . This is being done to see how the vertical offset Y_o and Surface velocity affects the motion of the micro-cantilever tip, and the horizontal driving force associated with that motion. Note only the vertical motion of the cantilever and the associated horizontal driving force will be shown because the horizontal motion is very small compared to the vertical motion as shown in Figure 51 and 52.

6 Discussion of Results

The goal of this research is to mathematically predict the Two-Dimensional dynamic response of a micro-cantilever and the corresponding horizontal driving force type force applied to the cantilever tip. The driving force for this analysis was assumed to be Lennard-Jones type atomic force as modeled in Figure 47. While several analytical situations are presented in the previous sections, we will now focus on the Two-Dimensional model of Figure 47 in our discussion. The assumptions made in the following discussion and analyses are:

$$\begin{aligned} f_{n_v} &= 20 \text{ kHz} & k_v &= 0.05 \text{ nN/nm} \\ f_{n_h} &= 90 \text{ kHz} & k_h &= 1.0125 \text{ nN/nm} \\ AS &= 0.4 \text{ nm} \end{aligned}$$

$$F_v = -\frac{6(2Y_o + 2v)B}{((X_o + V_s t + u)^2 + (Y_o + v)^2)^7} + \frac{3(2Y_o + 2v)A}{((X_o + V_s t + u)^2 + (Y_o + v)^2)^4} + k_v v \quad (80)$$

$$F_h = -\frac{6(2X_o + 2V_s t + 2u)B}{((X_o + V_s t + u)^2 + (Y_o + v)^2)^7} + \frac{3(2X_o + 2V_s t + 2u)A}{((X_o + V_s t + u)^2 + (Y_o + v)^2)^4} + k_h u \quad (81)$$

The only variables that are changed are the vertical offset (Y_o), and surface velocity, V_s . The time interval used is that for three atoms to pass under the tip of the micro-cantilever. Below are the three parametric cases:

Case 1 – $V_s = 500 \text{ nm/s}$ and 1000 nm/s for $Y_o = 0.75 \text{ nm}$

Case 2 – $V_s = 500 \text{ nm/s}$ and 1000 nm/s for $Y_o = 0.66 \text{ nm}$

Case 3 – $V_s = 500 \text{ nm/s}$ and 1000 nm/s for $Y_o = 0.5 \text{ nm}$

The time for the parameter study is the time required for the surface to travel a distance of two atomic spaces. The static vertical potential curves for each case are shown in Figure 53. These potential curves are most helpful in understanding the motion and horizontal driving force response of the tip. Refer to Appendix for Case 2 and Case 3.

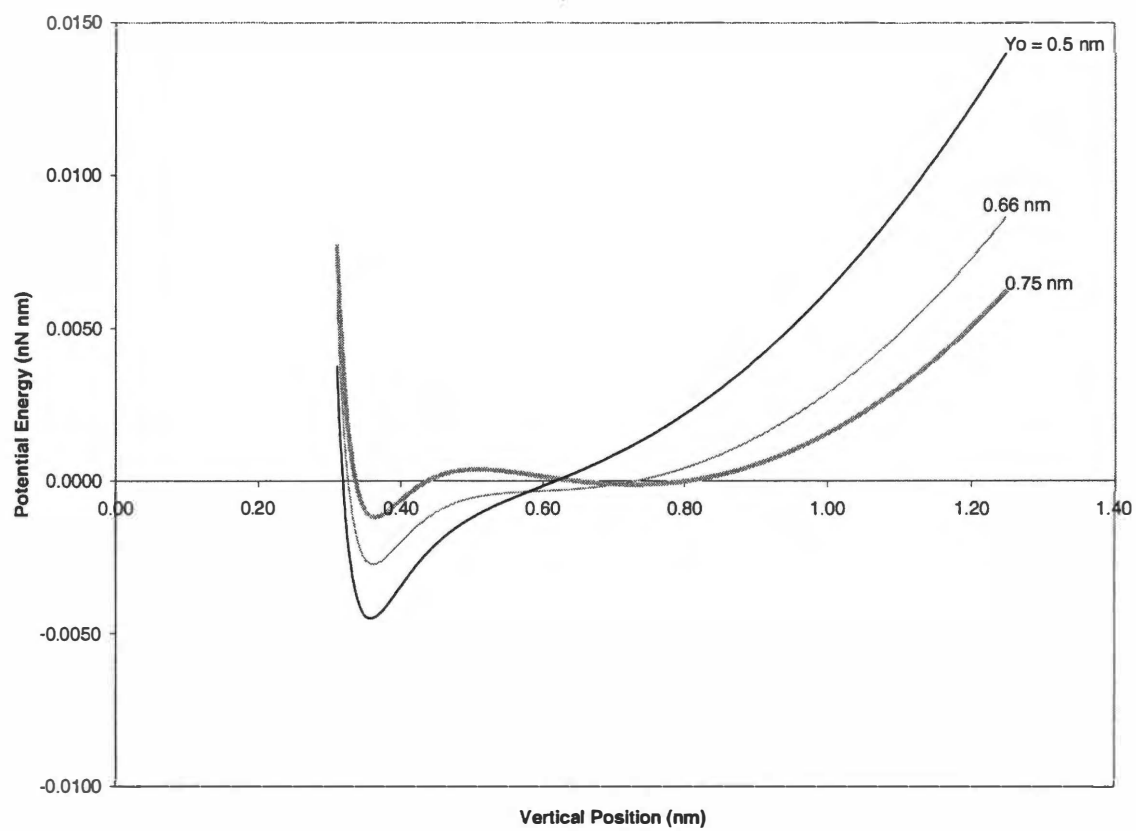


Figure 53: The total vertical potential for various Y_o values examined for a $k_v = 0.05 \text{ nN/nm}$.

Case 1

The parameters used for this case are a surface velocity (sliding velocity) of $V_s = 500 \text{ nm/s}$ & 1000 nm/s for a $Y_o = 0.75 \text{ nm}$. The results shown in Figure 54 show that the vibration is a free vibration the tip vibrates mainly in the spring's potential. The horizontal driving force the tip feels is the same as the horizontal static force between two atoms with a fluctuation riding the force due to the vertical natural frequency of the micro-cantilever beam as seen in Figure 55. Figure 56 and 57 shows that increasing the scanning velocity results in the time scale of the plot to change. The oscillations riding on the vibration are due to the vertical natural frequency of the micro-cantilever beam. Note the atoms cannot be seen in these plots.

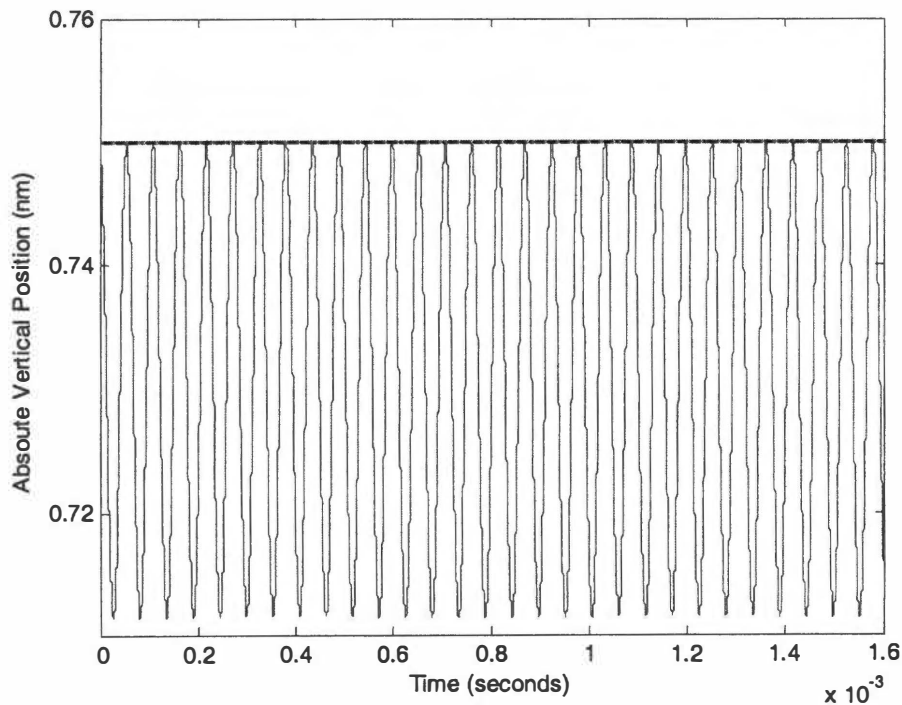


Figure 54: The absolute vertical motion of the micro-cantilever tip is based on the following $k_v = 0.5 \text{ nN/nm}$, $k_h = 1.0125 \text{ nN/nm}$, $AS = 0.4 \text{ nm}$, and $V_s = 500 \text{ nm/s}$, $Y_o = 0.75 \text{ nm}$.

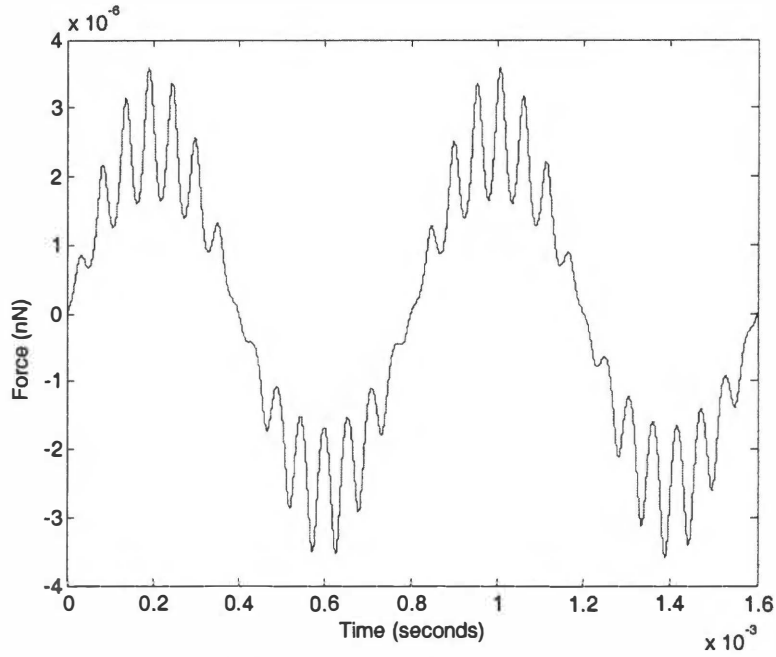


Figure 55: Horizontal force or driving force the tip of the micro-cantilever feels is based on the following $k_v = 0.5 \text{ nN/nm}$, $k_h = 1.0125 \text{ nN/nm}$, $AS = 0.4 \text{ nm}$, and $V_s = 500 \text{ nm/s}$, $Y_o = 0.75 \text{ nm}$.

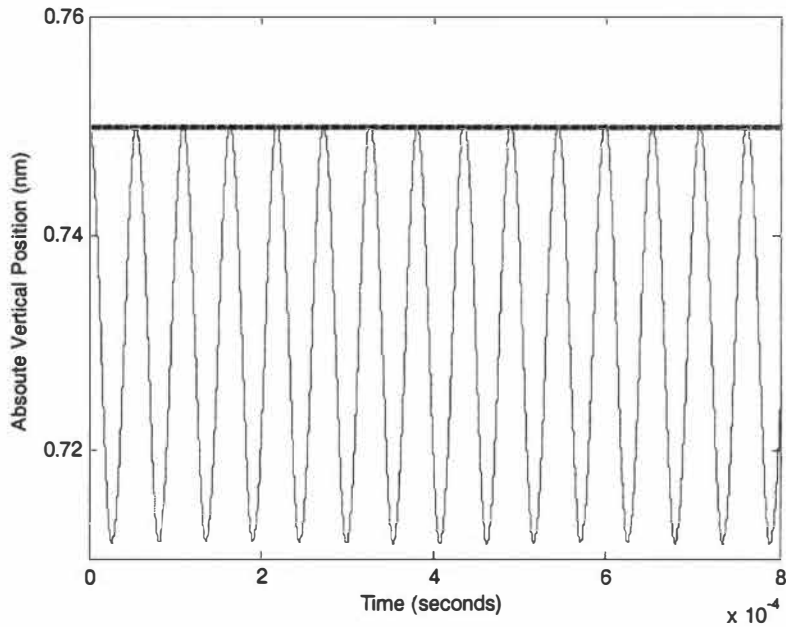


Figure 56: The absolute vertical motion of the micro-cantilever tip is based on the following $k_v = 0.5 \text{ nN/nm}$, $k_h = 1.0125 \text{ nN/nm}$, $AS = 0.4 \text{ nm}$, and $V_s = 1000 \text{ nm/s}$, $Y_o = 0.75 \text{ nm}$.

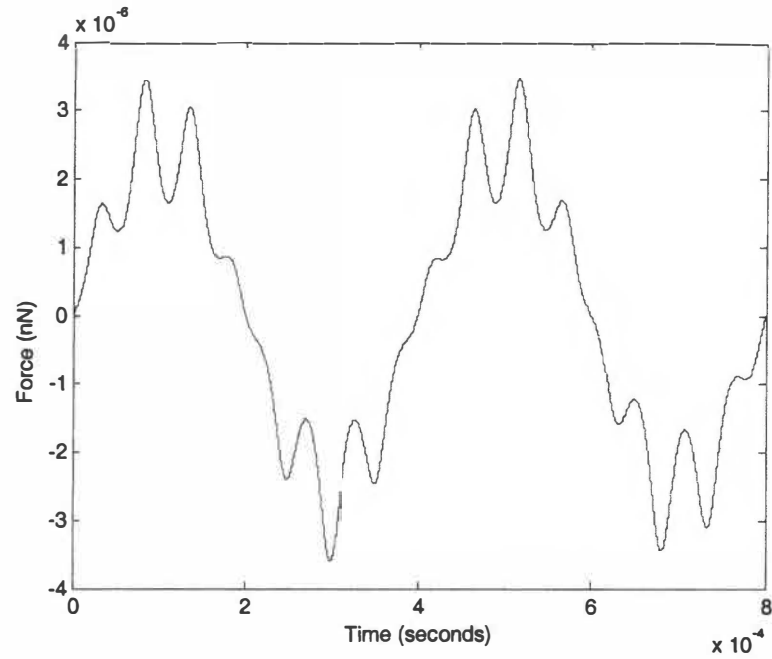


Figure 57: Horizontal force or driving force the tip of the micro-cantilever feels is based on the following $k_v = 0.5 \text{ nN/nm}$, $k_h = 1.0125 \text{ nN/nm}$, $AS = 0.4 \text{ nm}$, and $V_s = 1000 \text{ nm/s}$, $Y_o = 0.75 \text{ nm}$.

7 Conclusions

Micro-cantilever tips of the type used in atomic force microscopes (AFM) have elastic structural flexibility in both the vertical and horizontal directions. These two flexibilities can be defined in terms of spring constants; the spring constant for the vertical mode being smaller than that for the horizontal mode. These springs constant interact with the atomic potential field between the single tip atom and a row of surface atoms to generate tip motion in two dimensions. The associated atomic interactive forces are also dynamic.

The dynamic response of the tip depends greatly on the offset distance of the cantilever. It is only when the offset is roughly in the range of atomic spacing that horizontal driving becomes visible. The vertical potential diagram (Figure 53) is useful in picturing tip motion and horizontal driving responses. When the tip offset was just twice atomic spacing, tip motion and horizontal driving was predicted to be relatively small. However when tip offset is roughly equivalent to atomic spacing, tip motion and horizontal driving was predicted to be significant.

The time history of tip motion and horizontal driving with a large offset was regular and seemed to be dominated by the cantilever spring. Vibrations could be related to both natural frequencies of the vertical mode and frequencies associated with atomic spacing.

When the tip offset was equivalent to the atomic spacing the calculated tip motion and horizontal driving force became erratic. Further study is needed to explain these erratic predictions.

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List of References

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Appendix

Case 2 and Case 3

Case 2 and Case 3 presented special computational challenges. In these cases the repulsive force becomes a significant factor. These repulsive forces change considerably and more attention is needed to achieve a high level of confidence in the calculated responses.

Because the response for the calculations in Case 2 and 3 were somewhat erratic in comparison with that in Case 1, the responses were recalculated using smaller time steps. The response was essentially the same. Energy values over any time step were also checked. Since the system is conservative, there should be no change in the total energy over every time step. These calculations showed that the total energy with time is fairly constant as expected for a conservative system. The largest variation occurred in the repulsive part of the vibration cycle where the slope of the total potential is the steepest. It was decided to leave the calculations for Cases 2 and 3 as shown for completeness of the study.

Case 2

The parameters used for this case are a surface velocity (sliding velocity) of $V_s = 500 \text{ nm/s}$ & 1000 nm/s for a $Y_o = 0.66 \text{ nm}$ as plotted in Figure 58-61. The results shown in Figure 58 shows that the vibration is not a free vibration. The tip vibrates through the atomic and the spring's potential, which is non-linear. The noise seen riding the vibration is due to the cantilever's natural frequency. The horizontal driving force the tip feels has a similar pattern as that that is seen in the horizontal static force between two atoms with a fluctuation riding the force due to the natural frequency of the micro-cantilever beam and the non-linearity of the driving force as seen in Figure 59. Figure 60 and 61 shows that increasing the scanning velocity results in the period between atoms to decrease and the number of cycles of the vibration or noise riding on the main vibration decreases. The locations of the atoms are visible as the tip moves closer to the surface.

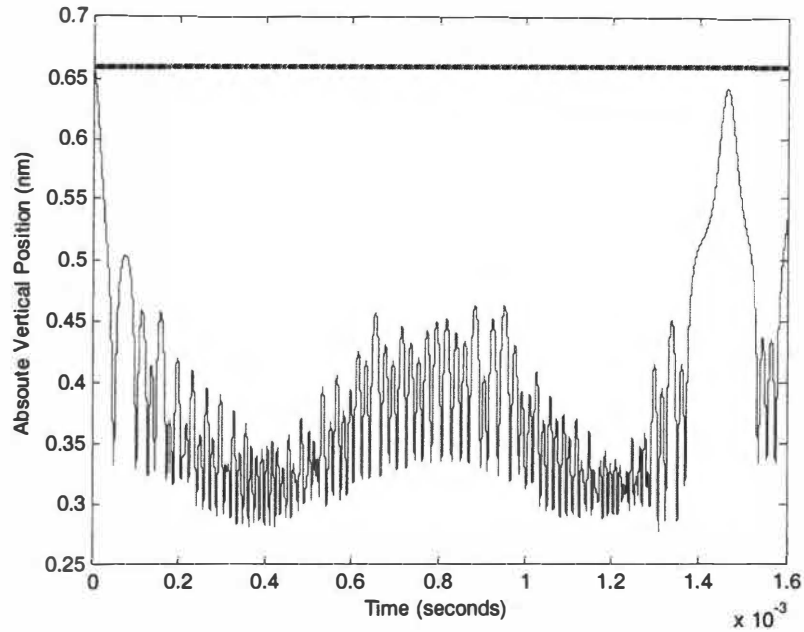


Figure 58: The absolute vertical motion of the micro-cantilever tip is based on the following $k_v = 0.5 \text{ nN/nm}$, $k_h = 1.0125 \text{ nN/nm}$, $AS = 0.4 \text{ nm}$, and $V_s = 500 \text{ nm/s}$, $Y_o = 0.66 \text{ nm}$.

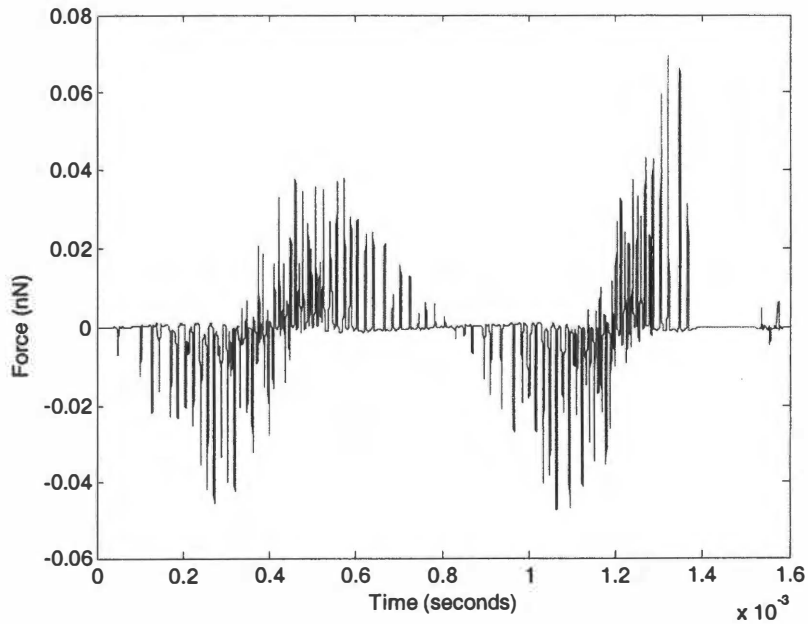


Figure 59: Horizontal force or driving force the tip of the micro-cantilever feels is based on the following $k_v = 0.5 \text{ nN/nm}$, $k_h = 1.0125 \text{ nN/nm}$, $AS = 0.4 \text{ nm}$, and $V_s = 500 \text{ nm/s}$, $Y_o = 0.66 \text{ nm}$.

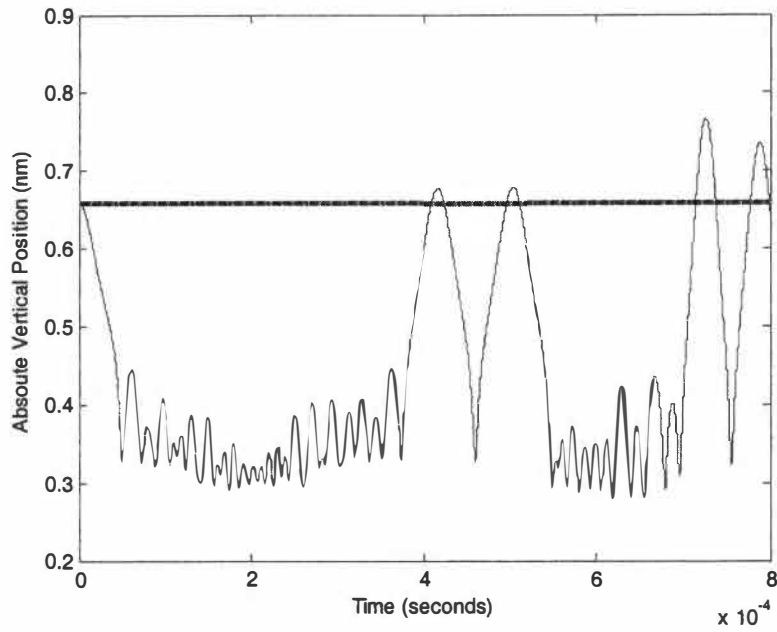


Figure 60: The absolute vertical motion of the micro-cantilever tip is based on the following $k_v = 0.5 \text{ nN/nm}$, $k_h = 1.0125 \text{ nN/nm}$, $AS = 0.4 \text{ nm}$, and $V_s = 1000 \text{ nm/s}$, $Y_o = 0.66 \text{ nm}$.

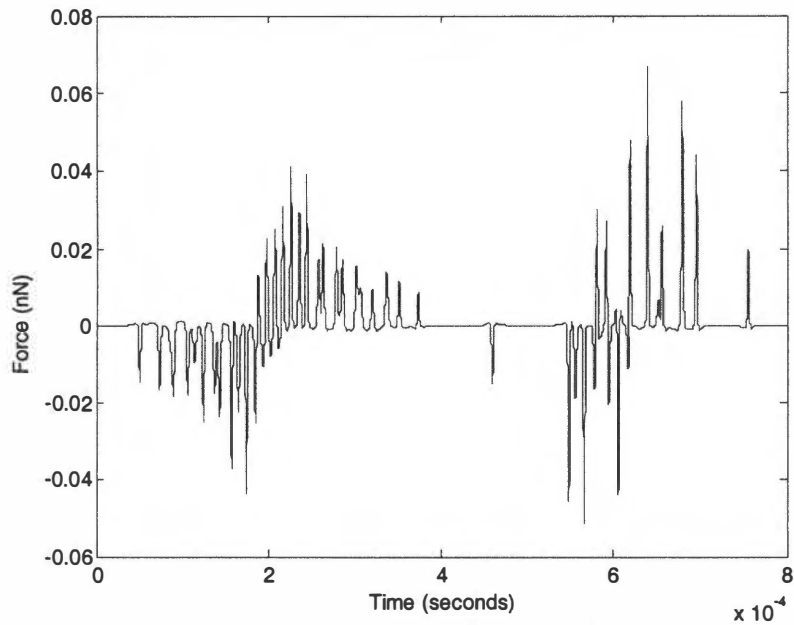


Figure 61: Horizontal force or driving force the tip of the micro-cantilever feels is based on the following $k_v = 0.5 \text{ nN/nm}$, $k_h = 1.0125 \text{ nN/nm}$, $AS = 0.4 \text{ nm}$, and $V_s = 1000 \text{ nm/s}$, $Y_o = 0.66 \text{ nm}$.

Case 3

The parameters used for this case are a surface velocity (sliding velocity) of $V_s = 500$ nm/s and 1000 nm/s for a $Y_o = 0.5$ nm as plotted in Figure 62-65. The results shown in Figure 62 show that the vibration is not a free vibration the tip because the tip vibrates through the atomic and the springs potential, which is non-linear. These results are similar to those seen in Case 2, but the number of cycles due to the natural frequency of the cantilever has increased. The horizontal driving force the tip feels has a similar pattern as that that is seen in the horizontal static force between two atoms with a fluctuation riding the force due to the natural frequency of the micro-cantilever beam and the non-linearity of the driving force as seen in Figure 63. Figure 64 and 65 shows that increasing the scanning velocity results in the period between atoms to decrease and the number of cycles of the vibration or noise riding on the main vibration decreases. The atoms are more visible as the tip moves closer to the surface compared to Case 1 and Case 2.

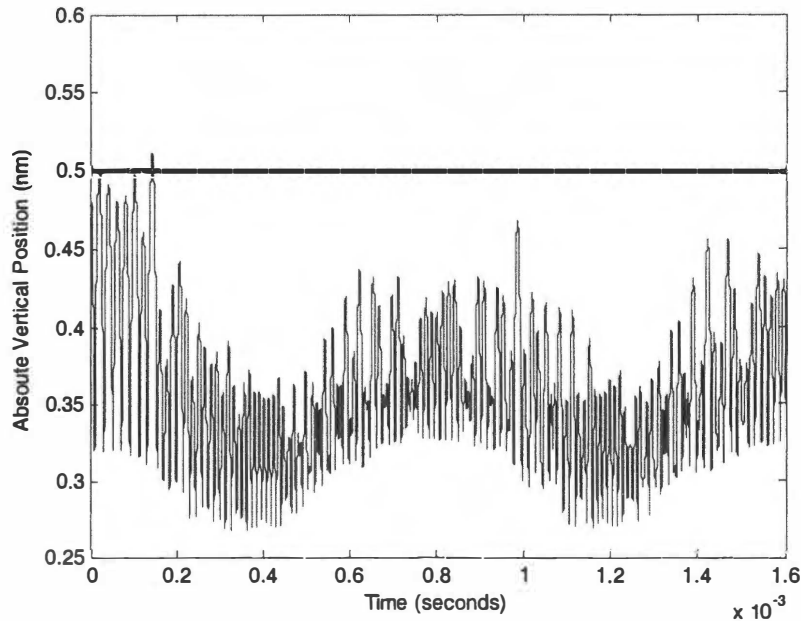


Figure 62: The absolute vertical motion of the micro-cantilever tip is based on the following $k_v = 0.5$ nN/nm, $k_h = 1.0125$ nN/nm, $AS = 0.4$ nm, and $V_s = 500$ nm/s, $Y_o = 0.5$ nm.

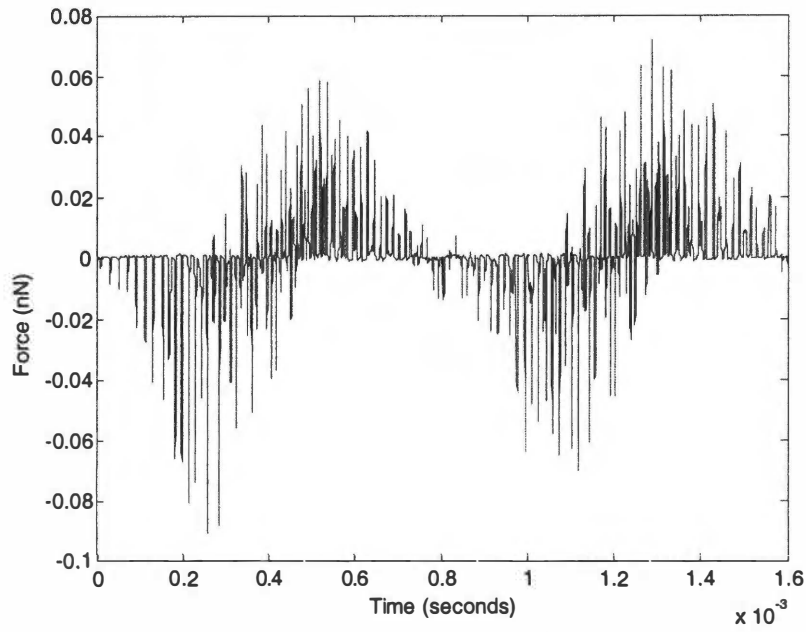


Figure 63: Horizontal force or driving force the tip of the micro-cantilever feels is based on the following $k_v = 0.5 \text{ nN/nm}$, $k_h = 1.0125 \text{ nN/nm}$, $AS = 0.4 \text{ nm}$, and $V_s = 500 \text{ nm/s}$, $Y_o = 0.5 \text{ nm}$.

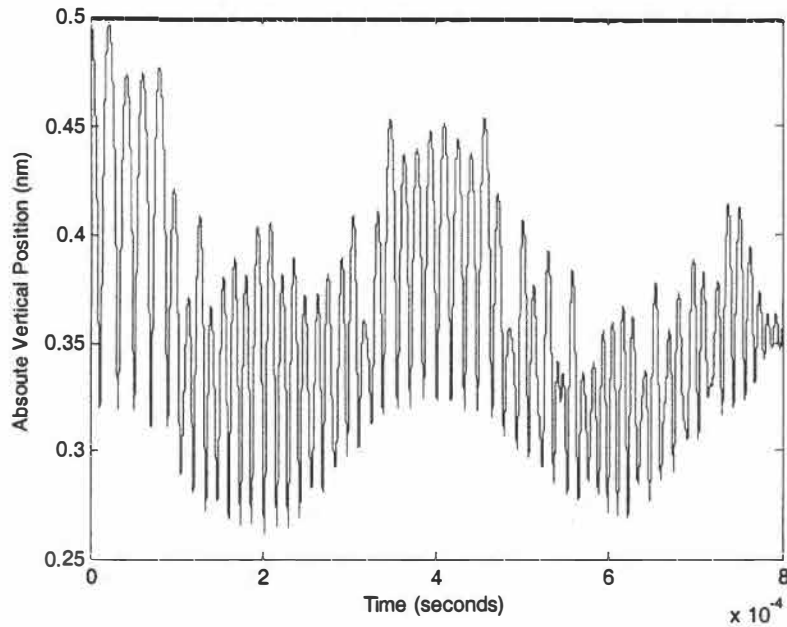


Figure 64: The absolute vertical motion of the micro-cantilever tip is based on the following $k_v = 0.5 \text{ nN/nm}$, $k_h = 1.0125 \text{ nN/nm}$, $AS = 0.4 \text{ nm}$, and $V_s = 1000 \text{ nm/s}$, $Y_o = 0.5 \text{ nm}$.

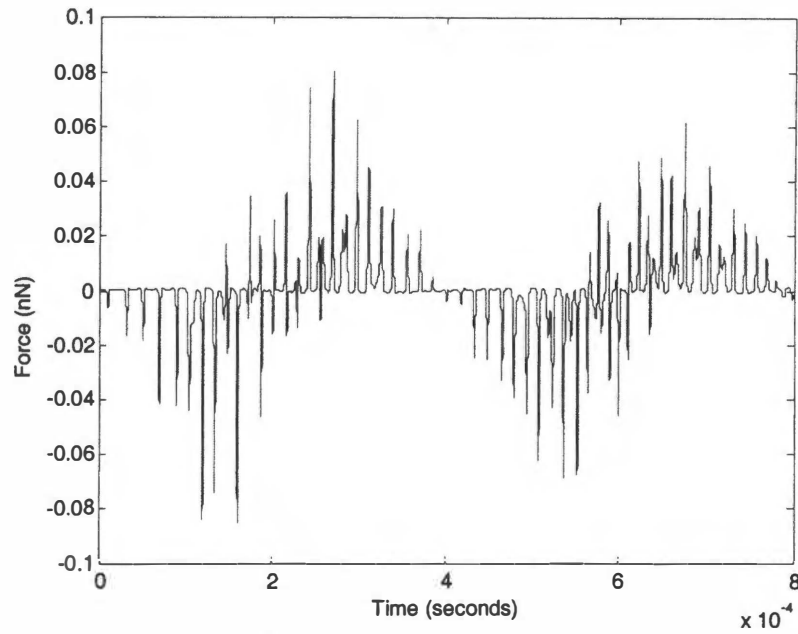


Figure 65: Horizontal force or driving force the tip of the micro-cantilever feels is based on the following $k_v = 0.5 \text{ nN/nm}$, $k_h = 1.0125 \text{ nN/nm}$, $AS = 0.4 \text{ nm}$, and $V_s = 1000 \text{ nm/s}$, $Y_o = 0.5 \text{ nm}$.

Vita

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