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Nano-scale Friction : A Review

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Frictional force is a resistant force that must be overcome to achieve relative motion between two components in contact. The economical and technological benefits of controlling friction and wear are tremendous. However, due to the complex nature of the phenomena, clear understanding of the mechanisms are yet to be achieved, particularly at the nano-scale where surface forces tend to dominate the tribological behavior of the system. In this paper the results of numerous theoretical, experimental, and numerical works on the fundamental mechanisms of friction at the nano-scale are reviewed. It is shown that friction coefficient values for nano-scale systems are quite varied depending on the conditions under which the system is investigated. As for the mechanism that causes friction at the nano-scale, interaction of the atoms plays a vital role. Furthermore, factors such as atomic radius, interatomic potential energy, and lattice parameters contribute to the degree of atomic interaction.

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1. Introduction

Friction is a force that resists the motion of two bodies in contact. Thus, in order to attain relative motion between the two bodies while in contact, frictional force must be overcome. The effects of friction can be found in every aspect of technology as well as nature. Due to its omnipresence and implication in everyday life, friction has been extensively investigated and researched over hundreds of years. The field that deals with friction is tribology. The word ‘tribology’ originated from ‘tribos’ which is a Greek word that means to rub. Tribology covers other related disciplines of friction, including wear and lubrication. In a broader sense, tribology covers all the phenomena related to relative motion of two contacting surfaces.

Since early civilization, efforts to control friction have been made. Wheel, for example, was invented to overcome friction between the carrier and the ground during transportation. Use of natural oil products to reduce friction can be tracked back thousands of years. Essentially, oil served as a lubricant that has been widely used even to this day. Traditional knowledge of tribology such as using liquid lubricant has been applied for long time before modern age without scientific considerations. Most of the early remedies for tribological problems were derived from everyday experiences and observations.

The research on friction conducted by Leonardo da Vinci in the 15th century is evidently the first scientific effort to better understand the nature of friction.[1] Also, it was not until the work by Reynolds in the 19th Century that a scientific theory for lubrication was proposed. Since then, countless other researchers have contributed to the vast literature on the topic of tribology and significant advances have been made over the years. Through these efforts, understanding of mechanisms of friction and wear has been steadily improving.

The most important motivation to achieve complete understanding of friction and wear mechanisms is ultimately to control these phenomena in various applications. The advantages that can be derived by controlling friction and wear are tremendous. The most obvious advantages lie in improved energy efficiency and life of the product. Hence, economic benefits of controlling these phenomena are quite profound. It has been reported that monetary value of tribological problems amount to as much as several percent of a nation’s GNP.[2,3]

Other than the economical benefits of controlling friction and wear, the technical implications are significant as well. For every moving component, the tribological issues become important. In some instances, friction can be the dominating factor in making the system work. Wear on the other hand is detrimental to the system function. It can cause early failure and other operational problems.

Therefore, the role of tribology in modern industry is critical and necessary to support the operation of all moving mechanical systems. To this end, continuous efforts are being made to better control the tribological phenomena in a variety of technologies.

The first step in controlling friction and wear is to understand the mechanisms behind these phenomena. The mechanisms are difficult to assess due to the complicated nature of the contact interface between two solid surfaces. The inevitable presence of asperities as well as altered surface chemistry due to environmental effects make it extremely difficult to determine the factors such as real contact area, contact stresses, and surface forces needed to estimate the frictional force. Nevertheless much progress has been made in understanding the major mechanisms of friction.

It is generally accepted that friction is caused by more than one mechanism in a given sliding system. Generally, frictional force arises due to two fundamentally different causes, namely one that is mechanical in nature and the other being chemical in its origin. In the case of mechanical cause of friction, plowing of the surface by hard particles or asperities is mainly responsible for generating the frictional force.[2,4,5-7] As for the chemical mechanism of friction, adhesion between surfaces of the two solids in contact is the cause of friction.[2,4,5,8] Another point to note is that tribological phenomena are heavily dependent on system parameters of the operating machine such as speed, temperature, load, and environment. As such, the dominating mechanism of friction depends on the system parameters

Tribological systems pose a wide range of dimensional scale. At the largest scale, geological stratum layers that are involved in earthquakes may be considered as a tribological system. The movement of the stratum occurs when the frictional forces between the layers are overcome by internal pressure inside the earth. At the smallest scale, relative motion of atoms at the interface of two materials would be a good example that involves frictional interaction. Owing to the vast difference in scale, the dominant mechanisms of friction and wear in macro-scale systems may be different from those of micro/nano-scale systems. In macro-scale, the tribological systems experience relatively large contact stresses and speeds. On the other hand, micro/nano-scale systems operate under relatively low loads and speeds. Particularly, the inertial effects that are prominent in macro-scale may be insignificant at the micro/nano-scale. Rather, surface forces often dictate the tribological interactions at small scales.[9,10] Since the ratio of surface area to volume increases drastically with decreasing dimension, various surface related phenomena such as adhesion, friction, surface tension, and stiction are critical to micro/nano-scale systems.

A major application of tribology in micro/nano-scale systems can be found in Micro/Electro-Mechanical-Systems (MEMS). MEMS components typically have dimensions in the range of 100 nm to 1 mm.[11] Microscopic mechanical components are fabricated using silicon-based materials to create a variety of devices such as sensors and micro-motors. The first MEMS device with moving components was reported in the 1980s. The device consisted of various moving elements such as gears, pin joints, and springs.[12] One of the major obstacles in adequate functioning of this device was the friction problem that is yet to be solved for the device to be utilized commercially. Another application where tribological phenomena at the micro/nano-scale become critical is the head/disk interface of a hard disk drive. The interaction between the slider, on which the head is embedded, and the disk media is critical to the reliability of the hard disk drive. Since magnetic spacing needs to be kept as low as possible to attain the high recording areal density, the flying height of the slider in today's hard disk drive is made to be well under 10 nm and the thickness of the surface protective layer is only a few nanometers thick.[13-15] Tribological optimization of the head/disk interface has been a major topic of research and development over the last couple of decades and has led to significant advancements in micro-tribology.[16,17]

Driven by the demands of applications such as MEMS and hard disk drives, micro/nano-tribology emerged as an important field within tribology since the 1980s and numerous researches have been conducted that made significant contributions to nano science and technology.[18] However, though many experimental and analytical works have been reported, clear understanding of the mechanism of friction and wear at the nano-scale is yet to be achieved. One of the reasons for such a lack of understand despite extensive research may be the fact that tribological interactions at the nano-scale tend to be extremely sensitive to the conditions under which the investigation takes place. Hence, repeatability and validity of the results are sometimes questionable and challenged. This point limits the use of tribological knowledge to advance the relevant technological applications. Scientists and engineers need to understand the fundamental aspects of nano-tribology, including the diversity in the results pertaining to its mechanisms. In this paper, theoretical models of nano-friction, various experimental results and numerical researches are reviewed with the aim to provide a comprehensive summary of significant research results regarding nano-friction.

2. Nano-scale friction

2.1 Early theories of friction

Friction is a natural outcome when two surfaces make contact and slide against each other. Frictional force which is the resistant force that acts to oppose the sliding motion occurs at the contact interface. Theories behind the nature of friction have been proposed by many researchers. The early models of friction concern the effects of asperities and roughness of a surface. All solid surfaces have many irregular asperities and these asperities interlock together when two surfaces come into contact. The interlocking of asperities at the sliding interface was proposed as the cause of friction by earlier researchers, Leonardo da Vinci, Amonton, and Coulomb.[7,8] Based on the existence of asperities, it was suggested that real contact area changes according to the normal load though the apparent contact area remains the same. The discovery of dependence of normal load and independence of contact area on friction was reported by Leonardo da Vinci and the theory was further extended by Amonton.[19,20]

In the early 20th Century, an atomic-scale model of friction was proposed that laid the foundation for understanding nano-friction. Tomlinson (1929) reported an atomic friction model that was totally different from what was understood about friction at that time.[21] Tomlinson's model of friction was based on the assumption that surface was atomically smooth without any asperity. However, since atoms were modeled as spheres, the surface topography was not perfectly flat but consisted of protrusions corresponding to the radius of the atoms. The spacing between the protrusions was represented by the lattice constant or equivalent distance between the atoms in solid state. For such a solid surface model Tomlinson speculated that when a counter surface is slid on top interference between the atoms occur in the sliding direction as illustrated in Fig. 1. Fig. 1 shows a single atom (Atom 1) sliding on a surface with multiple atoms (Atom 2). It was suggested that friction between the two groups of atoms could be represented by a spring-like interaction that undergoes stretching and contraction as the atoms slide against each other. When Atom 1 is located between two atoms of the surface, it is stable and the potential energy is minimized. This state can be viewed as a state when the spring is in its equilibrium position or length. With further movement of Atom 1, the spring is stretched to cause an increase in the potential energy. The potential energy is maximized when Atom 1 position is aligned on top of Atom 2. The potential energy is released as Atom 1 is pushed to the next stable position along the surface.[21-24] This model is regarded as the first explanation of atomic-scale friction. Though the model did not describe the atomic-scale friction fully accurately, it provided a useful insight for the behavior of friction such as stick-slip.

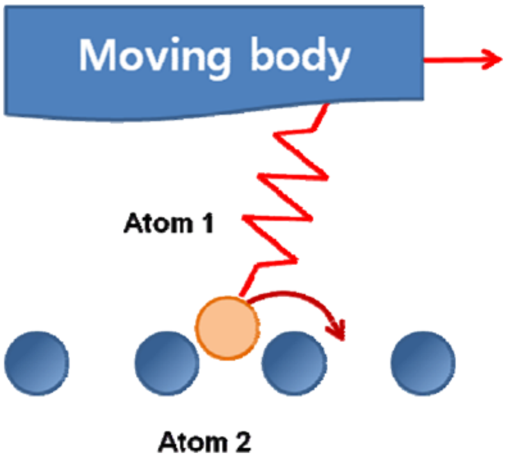

Fig. 1 Schematic of Tomlinson atomic friction model. The surface is represented as an atomically smooth surface with protrusions corresponding to the atomic radius. Frictional behavior is described by interference between Atom 1 and Atom 2 as they slide against each other [adapted from 21]

Another theoretical model for atomic-scale friction is the Frenkel-Kontorova (FK) model (1938). The Frenkel-Kontorova model is a 1-dimensional model that consists of interaction between the substrate atoms with sinusoidal potential and a chain of surface atoms linked by spring as shown in Fig. 2. The surface atoms are connected to each other by harmonic springs and a periodic potential force is applied to the atoms. The model is useful to derive the adsorption characteristics during the frictional interaction of the atoms on an atomically flat surface. The model was further discussed and extended by Frank and van der Merwe (1949) and Bak and Pokrovsky (1981).[24-26] However, Weiss and Elmer (1995) proposed that the model had a deficiency. They suggested that in the FK model, there was no connection between the atoms and the sliding body. Therefore, Frenkel-Kontorova-Tomlinson (FKT) model that combines the FK model with the Tomlinson model was proposed. The model also provided a case for wearless frictional interacton and described the effect of commensurability on the frictional behavior.[27,28] As shown in Fig. 2, when the two layers are commensurate, atoms of the top layer are spatially matched with the atoms of the bottom layers. In this case contribution of each atomic pair to the total frictional force is maximized, thus leading to a relatively high friction. On the other hand, when the two layers are incommensurate the frictional force of each atomic pair may cancel out among the other pairs, thus leading to a low frictional force.

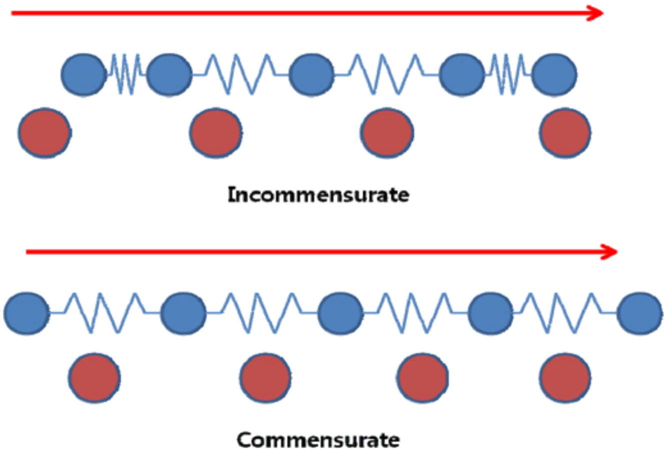

Fig. 2 Schematic of Frenkel-Kontorova model. The atoms are linked by harmonic springs and a periodic potential force is applied to the atoms [adapted from 25]

Quite some years after the FKT model was presented, Bowden and Tabor (1954) proposed the adhesion model that is illustrated in Fig 3 as the major mechanism of friction. They suggested that small junctions of asperities are formed due to contact pressure and adhesion. The combined area of all the junctions essentially represents the real contact area. According to the model, frictional force, F_r, is proportional to the real contact area as described by the following equation:

$$F_r = \sigma A_r$$

where σ is the shear strength of the junction and A_r is the real area of contact. The frictional force is decided by the shear strength which is an intrinsic property of the contact interface and the real contact area. The model suggests that the real contact area is quite different from the apparent contact area and the static frictional force is dependent on the real contact area. In the model, the adhering asperities are formed as normal load is applied and friction is caused during relative motion by loss of energy due to plastic deformation of the asperities.[29]

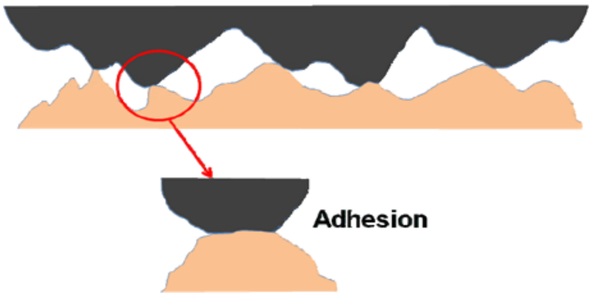

Fig. 3 Schematic of adhesion model proposed by Bowden and Tabor. Asperity junctions form due to contact and adhesion. Frictional force is generated as the junctions break at or near the contact interface [adapted from 29]

2.2 Experimental works

Experimental research to examine the frictional characteristics at the atomic-scale has been conducted for the past two decades. It is well known that frictional behavior cannot be generalized by a few factors such as normal load, surface roughness, speed, and material type of the tribological system. Other conditions such as temperature, humidity, and even sliding history can affect the tribological phenomena significantly. Particularly at nano-scale, the tribological behavior tends to be more sensitive to the state of outermost layer of the surface region. Thus, contamination layer, adsorbed gas, capillary junctions, and oxide layer become more important at small scales. This is because at nano-scale the contact forces are often too low for the asperities to penetrate the surface layers and the magnitude of the surface force may be comparable to the frictional force. Therefore, well-controlled specimen and experimental conditions should be prepared to guarantee the reliability of the results of nano-scale friction experiments.

Conventional testers used for friction experiments do not have the resolution to measure the frictional force at the atomic level. The development of Atomic Force Microscope (AFM) in mid 1980s, which was a breakthrough in the field of surface science, made it possible to probe into nano-scale friction experimentally. The functions of an AFM are based on atomic force that is generated when a very sharp stylus is placed in proximity to a surface. The interaction of atoms at the tip of the stylus and the top surface layer of the specimen generates either attractive or repulsive force that can be monitored using an ultra-high sensitive force sensor as the stylus scans the surface with sub-nanometer resolution. Using this device, surfaces forces such as adhesion and friction can be measured with fraction of a nano-Newton resolution.[19]

Characteristics of atomic-scale friction were first reported by Mate et al. in 1987.[30] The research was conducted with an AFM and the results showed the frictional interaction between a sharp tungsten tip and a graphite substrate. Very small loads ($< 10^{-4}$ N) were used in the experiment and the average friction coefficient was found to be 0.012. Also, the experiment clearly demonstrated the stick-slip behavior of atomic-scale friction with a period corresponding to the lattice constant of graphite. This result was consistent with the atomic friction model of Tomlinson.

Following the seminal work published by Mate et al., numerous other experimental works were carried out to assess the nature of atomic-scale friction. Akamine et al. (1990) obtained an AFM image of Au on mica surface and a saw tooth shaped stick-slip behavior was observed when 10^{-7} N normal load was applied.[31] Fujisawa et al. (1993) performed experiments with a Si_3N_4 tip and mica substrate to investigate the atomic-scale stick-slip motion. They changed the scan direction to investigate the dependence of lattice orientation on vertical and lateral forces. According to the experiment, a square-wave shaped vertical force and a saw tooth shaped lateral force (or vise versa) were observed during the stick-slip motion of the tip as shown in Fig. 4. Such behavior was attributed to the zigzag motion of the AFM tip as illustrated in Fig. 5.[32]

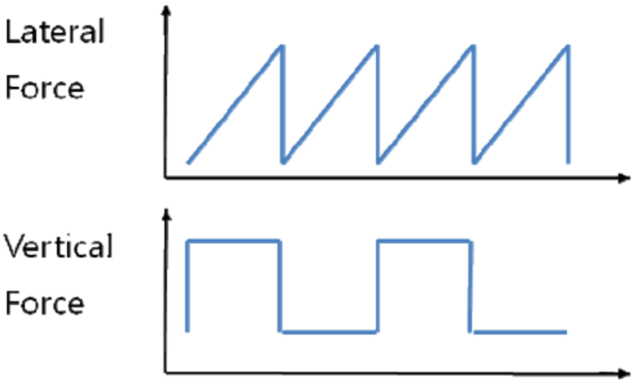

Fig. 4 Schematic of lateral and vertical forces in 2-dimensional atomic-scale stick-slip behavior [adapted from 32]

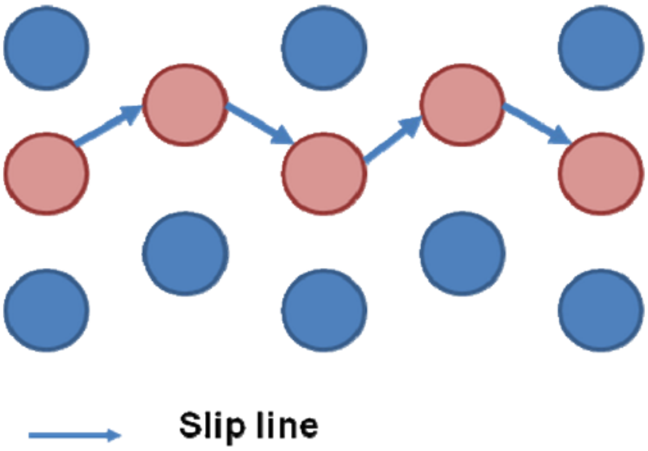

Fig. 5 Schematic of zigzag motion of the AFM tip in 2-dimensional atomic-scale stick-slip model [adapted from 32]

Ruan and Bhushan (1994) used an AFM to investigate the effect of surface roughness on the tribological characteristics of graphite using a Si_3N_4 tip. It was found that friction coefficient varied with respect to roughness of the substrate. The friction coefficient was below 0.01 and 0.03 for RMS roughness of about 10 nm and 140 nm, respectively. This outcome was attributed to the loss of orientation of the substrate with increasing roughness.[33]

Jiang et al. (1995) conducted friction and indentation experiments with a diamond tip and hydrogenated carbon film coated on silicon wafer.[34] Hydrogenated carbon film was coated to a thickness of 25 nm on a silicon substrate. They obtained a friction coefficient of 0.02 using an AFM. Indentation tests were also carried out to measure the hardness of the film with respect to indentation depth. The results showed that hardness increased with indentation depth up to the maximum depth of 14 nm. Considering that the thickness of the film was 25 nm, the substrate effect was likely to have occurred beyond the depth of about 10 nm. When indentation test was performed on a single crystal silicon without any coating the hardness was found to decrease with indentation depth.[35] The change in hardness was attributed to variation in defect density.

The works of Bhushan and Kulkarni (1996)[36] and Tambe and Bhusan (2004)[9] showed the difference in frictional behavior with respect to scale. They reported that friction coefficient decreased with decrease in scale. The results showed that while the friction coefficient of Si (111) in macro-scale experiment conducted with a load of 1 N was approximately 0.6, the value decrease by almost 10 times to 0.05 in nano-scale experiment conducted with a load of 1~15 μN. This drastic change in friction coefficient was due to the change in the mechanism of friction as the contact condition was altered even for the same pair of material system.

Tambe and Bhushan (2005) reported the dependence of velocity on the frictional behavior in nano-scale.[37] Various materials such as bare silicon with native oxide, DLC and Z-15 coatings on silicon wafer were used in the experiments. In the case of bare silicon and Z-15 coating, frictional force initially decreased from 20 nN to 15 nN and 5 nN to 3 nN, respectively, with increase in sliding velocity from 5 to 1000 μm/s due to the formation of meniscus. Meniscus force of bare silicon and Z-15 coated surface was caused by condensed water molecules and molecules of Z-15, respectively. However, at higher velocities above a critical value, the frictional force increased due to insufficient time to form a meniscus at the asperity contact junction. In the case of DLC, the frictional force decreased above a certain sliding velocity. This was attributed to phase transformation of the DLC film.

Bhushan and Sundararajan (1998) investigated the effects of relative humidity and tip radius on nano-frictional behavior. The primary purpose of changing the tip radius was to vary the contact area in the friction experiments. The results showed that friction coefficient increased with humidity and contact area.[38] Nair and Zou (2008) investigated the effects of surface texturing on the frictional behavior of amorphous silicon. Texture was formed on the specimen surface by etching. Friction tests were carried out with a 100 μm radius tip. It was found that friction coefficient could be reduced from 0.5 to 0.05 by nano-texturing.[39] Sung et al. (2003) carried out friction tests with micro-grooved silicon surfaces. Both micro-tribotester and AFM were used to investigate the micro/nano frictional behavior. It was reported that contact angle between the groove and the pin affected the frictional characteristics significantly. High contact angle led to a sudden increase in the frictional force due to interlocking mechanism. The effect of slope between the tip and the asperities on the frictional behavior was also reported.[10] These works suggest that frictional behavior at micro/nano scale is very much dependent on the surface structure and topography. Furthermore, the contact geometry between the tip and the surface such as area and orientation of the contacting angle affect the frictional force significantly.

Along with nano-scale friction, wear at nano-scale has also been extensively investigated. Chung et al. (2007) investigated the wear characteristics of materials widely used in MEMS application under very small loads in the order of 100 μN. Wear tests were carried out with micro bushings fabricated on silicon sliding against a silicon wafer. The results showed that the wear coefficient was in the range of 0.8~5.2 x 10^{-7}.[40] In another work the tribological behavior of PZT thin film at nano-scale was obtained. By using an AFM, hardness, elastic modulus, friction coefficient, and wear rate were obtained for PZT thin film. The friction coefficient and wear rate was in the range of 0.1 to 0.2 and 2.4 x 10^{-8} to 4.5 x 10^{-8} mm^3/N cycle, respectively.[41] Chung et al. (2008) also obtained the friction and wear coefficients of ZnO nanowires under extremely small loads in the range of 50 to 150 nN. The friction and wear coefficients were around 0.25~0.3 and 0.006~0.162, respectively.[42]

2.3 Numerical analysis

With the advancement of computational capability the use of computer simulation to investigate atomic-scale interactions has been steadily increasing. Over the years, numerical methods have been employed in nano-tribology to predict its behavior at the atomic-scale. Since continuum mechanics is not valid for nano-scale analysis, conventional simulation method such as Finite Element Method (FEM) cannot be effectively utilized for nano-tribological studies. Therefore, analytical methods such as Molecular Dynamics (MD), Monte Carlo (MC), and Ab initio calculations are favored in atomic-scale analyses.[43]

MD method is useful to simulate the nano-tribological characteristics for various materials and contact conditions. MD simulation is a powerful technique to gain insight for nano-scale phenomena since it provides good visualization effects as shown in Fig. 6. Since MD simulation is based on classical mechanics, quantum effects may be ignored and hence the calculation speed is relatively fast. Furthermore, various parameters such as force, energy, temperature, and pressure can be obtained during the simulation. Fig. 7 shows an example of a frictional force data obtained from MD simulation. The results show the fluctuating nature of the forces involved in nano-scale interaction. The friction and normal forces are in hundreds of nN range.

Ab initio approach in the analysis of atomic-scale phenomena deals with quantum physics. The technique is used to investigate surface reconstructions, electronic energy, and also to derive parameters of empirical potentials. However, due to much more extensive calculation compared with MD simulation, Ab initio approach only treats a few atoms in the analysis.[4,44] With improvements in computing capability and techniques, various hybrid simulation methods are applied to simulate nano-scale phenomena. For example, a hybrid technique that combines MD and FEM simulations to investigate the characteristics of thin film lubrication was reported by Sham (1997).[45]

Kim and Suh (1994) performed a 2-dimensional MD simulation to investigate the atomic-scale frictional behavior using Lennard-Jones potential function. The simulation results showed clear evidence of stick-slip behavior with a period corresponding to the lattice constant of the substrate. The average friction coefficient was 0.05. They also calculated the increase in system temperature due to atomic-scale frictional interaction.[46] Sorensen et al. (1996) reported simulation results of atomic-scale friction under various conditions. Copper tip and substrate were used in the simulation and stick-slip behavior was also observed. The results further showed a decrease in frictional force from 2.2 to 1.5 nN with an increase in sliding velocity from 1 to 20 m/s.[47] Lia et al. (2001) also carried out simulation regarding stick-slip interaction of Ni-Al alloy. They found that the period of stick-slip was same as the lattice constant of Ni-Al alloy.[48]

Nano-friction is of great concern in the field of nano-machining since the frictional interaction between the tool and the workpiece dictates the machining characteristics. Belak and Stowers (1990) performed an MD simulation of orthogonal cutting process.[49] The atomic interaction between the atoms of the tool and the workpiece could be better understood from the simulation results. Cagin et al. (1999) investigated the nano-frictional characteristics for two flat diamond specimens sliding under contact. The results showed that the friction coefficient value was in the range of 0.01 to 0.25 and the value changed with respect to sliding direction.[50] Komanduri et al. (2000) performed a cutting simulation of silver substrate with respect to scratch direction. It was found that as the crystal orientation of the substrate was varied the friction coefficient, scratch hardness, and indentation hardness varied from 0.6~0.8, 15~21 GPa, and 3~5 GPa, respectively.[51] Wu et al. (2004) simulated the nano-machining process of silicon using a diamond tool. In the simulation, phase transformation of silicon due to high pressure during machining was found.[52] Yang and Komvopoulos (2005) investigated the effects of velocity, tip size, and shape of the tool on the frictional behavior. The results showed an increase in frictional force from 20 nN to 30 nN as sliding velocity increased from 1 to 100 m/s.[53]

Nano-friction of organic thin films commonly used for stiction and friction reduction of precision micro-systems has also been a topic of MD simulation. Tupper and Brenner (1994) carried out simulation on friction between two layers of SAM coated on gold surfaces. Compression characteristics of SAM and interaction between the two surfaces coated with SAM molecules were investigated in the simulation. The results showed the dependence of frictional force and normal load, and furthermore, it was demonstrated that Amonton's law was valid for nano-scale friction.[54] Lan and Zhang (2004) reported on the interaction between nano-scale tip and thin film which was similar to the model investigated by Tupper et al.[55] Zhang and Jiang (2002) also presented the frictional behavior of SAM molecules on Si (111) with respect to relative humidity. According to the simulation, friction coefficient of hydrophilic surface decreased from 0.5 to 0.2 as relative humidity increased from 15 to 80%.[56] Tanaka et al. (2003) performed simulation on the frictional behavior of Perfluoropolyether (PFPE) coating with respect to normal load. The results showed that friction coefficient decreased from 0.8 to 0.2 when the normal pressure was increased from 0.1 x 10^9 to 2.0 x 10^9 Pa. Stick-slip behavior and fluctuation of frictional force at high load were also observed in the simulation.[57] Sung and Kim (2005) reported the wear characteristics of Hexadecanethiol (HDT) coated on a silicon substrate. According to the result, the width of wear track increased with scribing speed and it was affected more by the tip shape rather than the tip size.[58]

Atomic-scale simulations have been widely used in nano-tribology research as discussed above. The simulation methods are useful to gain insight for nano-scale interactions and obtain quantitative results for various system models and operating conditions. However, there are still several problems that need to be tackled to obtain simulation results that are closer to the real world. One of the limitations of concern is in regard to the simulation scale. Despite relatively fast processor speed and efficient algorithm the number of atoms that can be handled realistically is still insufficient for complex system simulation. Also, the potential functions need to be further developed so that a larger spectrum of materials can be treated in the simulation. These limitations of numerical simulations are expected to be overcome in the future with the development of superior processors and more sophisticated algorithms.

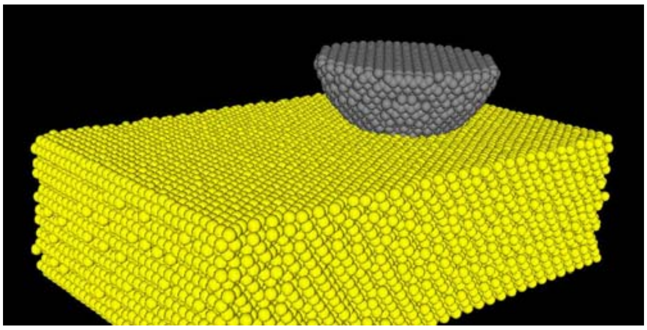

Fig. 6 Schematic of model for molecular dynamics simulation of nano-frictional interaction consisting of approximately 50000 atoms of Si tip and Ag substrate

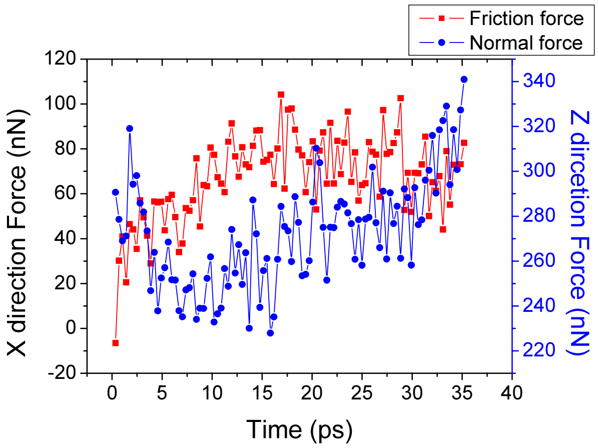

Fig. 7 Example frictional force obtained from MD simulation during ramp loading in hundreds of nN range

3. Summary

Tribological issues are encountered in almost all situations where relative motion occurs between two components in contact. Friction leads to unwanted energy consumption and wear limits the life of a product. Thus, by controlling friction and wear tremendous economic and technical benefits can be derived. However, due to the complex nature of these phenomena the ability to fully control their behavior is still lacking. In order to achieve this objective a clear understanding of the mechanisms of friction and wear must be achieved.

In this paper selected literature on nano-friction and related

Table 1 Summary of experimental results on nano-tribology

Year	Researcher	Experimental condition	Specimens	Key Results
1987[30]	Mate et al.	* Normal load < 10^{-4} N * AFM * Ambient air	Tungsten tip, Graphite substrate	Periodic stick-slip was observed Average friction coefficient : ~ 0.012
1990[31]	Akamine et al.	* Normal load : 10^{-7} N * AFM	Si tip Au(111) on mica surface	Periodic stick-slip was observed Average friction coefficient : 0.05
1993[32]	Fujisawa et al.	* Scan rate : 0.47 Ǻ/s ~ 120 Ǻ /s * AFM was used * Normal load : ~6.5 x 10^{-9} N * Various scan direction (0°, 60°, 90°, 180°, 240°, 270°)	Si_3N_4 tip Mica substrate	Stick-slip phenomenon with respect to scan direction 2 dimensional stick-slip
1994[33]	Ruan et al.	* AFM and FFM (Friction force microscope) * 50 x 50 nm^2 ~ 4 x 4 μm^2 scan area * Normal load : 42 nN * Scan speed : 1 μm/s	Si^3N^4 tip Highly oriented pyrolytic graphite substrate	Average friction coefficient : 0.03 Friction coefficient varied with respect to surface roughness
1995[34]	Jiang et al.	* FFM * (2~6) x (2~6) μm^2 scan area * Normal load : 20~200 μN * Indentation depth : 5~100 nm	Diamond tip Hydrogenated carbon thin film (25nm) on Si(100) Concentration of hydrogen : 2, 28 and 40%	Friction coefficient with respect to hydrogen concentration : 0.02~0.04 Low concentration of hydrogen was better for wear and friction For 2% hydrogenated film, hardness wrt indentation depth of 5, 9, 12, 14 nm was 9, 10, 10.5, 12.5 GPa, respectively
1996[36]	Bhushan et al.	* Scan length : 8 μm * Scan speed : 800 nm/s * Normal load : 0~40μN	Diamond tip Si_3N_4 tip Si(111) substrate SiO_2 substrate Polished diamond substrate	Macro scale friction coefficient : Si : 0.18~0.6 SiO_2 : 0.19~0.21 Polished diamond : 0.07 Micro scale friction coefficient : Si : 0.05~0.2 SiO_2 : 0.04~0.08 Polished diamond : 0.023~0.11
1997[35]	Ruan and Bhushan	* Normal load : 0.2~15 mN (for measuring hardness) * Normal load : 10 mN (for friction)	Undoped and doped Si(100) Undoped and doped poly Si wafer Diamond tip (radius : 20 μm) Sapphire ball (Radius : 3 mm)	Si(100) hardness : 13 GPa at load : 0.2 mN 11.9 GPa at load : 15 mN Friction coefficient : 0.05~0.1 with diamond tip 0.2~0.6 with sapphire ball
1998[38]	Bhushan and Sundararajan	* AFM, FFM * Tip radius 0.05~14 μm * 0~80% RH * Normal load : 50~250 nN	Si_3N_4 tip SiO_2 tip Si (100) Si (111)	Friction coefficient increased with tip radius and relative humidity : 0.05~0.13
2004[9]	Tambe et al.	* 20 ± 2 °C , 50± 5% RH * 20~125°C, 0~80% RH for measurement of adhesive force * Velocity : 4~720 μm/s * Scan size : 2 ~ 1000 μm	Si_3N_4 tip (radius 30~50nm) Si (100), PDMS, PMMA, DLC, Z-DOL, Z-15, HDT (Self-assembled monolayer)	Friction coefficient decreased with scale Si : 0.5 → 0.05 DLC : 0.19 → 0.03 HDT : 0.15 → 0.02 Z-DOL : 0.23 → 0.03 Z-15 : 0.06 → 0.01 PMMA : 0.2 → 0.06 PDMS : 0.3 → 0.1

Year	Researcher	Experimental condition	Specimens	Key Results
2005[37]	Tambe et al.	* AFM * Normal load : 70 nN * Scan velocity : 10 µm/s ~ 1 mm/s	Si_3N_4 tip Si(100) substrate DLC on Si HDT on Au/Si Z-15 on Si	Friction varied with velocity : Si(100), Z-15 sample : Initially decreased then, increased with velocity DLC sample : decreased above a certain sliding velocity
2007[40]	Chung et al.	* Nano friction tribo tester * Normal load : 100 µN * Sliding distance : 5.6~187 km * Diameter of bushing : 6~30 µm	Microbushing on Si (100), Silicon oxide, Silicon nitride, Polysilicon Si (100) wafer	Wear coefficient : Si (100) : 2.8 x 10^{-7} Silicon oxide : 5.2 x 10^{-7} Silicon nitride : 8.0 x 10^{-8} Polysilicon : 3.3 x 10^{-7}
2007[41]	Chung et al.	* AFM * Normal load : 0.1~ 3 µN and 5~10 µN * Thickness of PZT thin film : 120 nm	PZT thin film Pt/Ti/SiO2/Si (100) substrate for deposition of PZT thin film	Hardness of PZT thin film : 6.9~9.3 GPa Elastic modulus : 151~175 GPa Wear rate : (2.4–4.5)×10^{-8} mm^3/N
2008[42]	Chung et al.	* AFM * Radius of ZnO nanowire : 75±18 nm * Normal load : 50~150 nN * Scan speed : 2 µm/s * Scan area : 2x2 µm^2 * Relative humidity : 30%	Vertically aligned ZnO nanowire on saphire Diamond coated silicon probe tip	Wear coefficient of ZnO nanowire : 0.006~0.162 Friction coefficient : 0.25~0.3
2008[39]	Nair et al.	* 40% RH * Normal load : 75~1500 µN * Nano texture formed on the surface by etching process	Diamond tip Aluminum induced crystallization of amorphous silicon substrate	Friction coefficient of textured sample : 0.05~0.1 Friction coefficient of smooth sample : 0.12~0.5

Table 2 Summary of numerical analyses results on nano-tribology

Year	Researcher	Simulation condition	Used material	Results
1994[46]	Kim and Suh	* 2D scanning of atoms * Lennard-Jones potential		Stick-slip frictional behavior Friction coefficient : 0.05
1996[47]	Sorensen et al.	* 3175 atoms * Contact area : 140 Å^2	Copper probe tip Copper substrate	Stick-slip frictional behavior Decrease of frictional force from 2.2 to 1.5 nN as sliding velocity increased from 1 to 20 m/s Increase of friction force with contact area
2001[48]	Lia et al.	* EAM potential * 12000 atoms	Ni-Al alloy	Stick-slip frictional behavior Period of the stick-slip was same as the lattice constant of Ni-Al alloy
1999[50]	Cagin et al.	* Brenner's potential	Bare diamond Hydrogenated diamond	Dangling bond of surface caused higher friction force Different friction coefficient according to sliding direction
2000[51]	Komanduri et al.	* Morse potential * Various cutting directions	Single crystal aluminum	Different hardness and friction coefficient according to crystal orientation (Indentation hardness : 3~5 GPa) (Scratch hardness : 15~21 GPa) (Friction coefficient : 0.6 ~ 0.8)
2004[52]	Wu et al.	* Tersoff potential	Single crystal silicon Diamond cutting tool	During cutting process, phase transformation of silicon was found due to high pressure
2005[53]	Yang and Komvopoulos	* Morse potential * Lennard-Jones potential * Approximately 20000 atoms	Diamond tip Copper substrate	Stick-slip frictional behavior Increase of friction force from 20 nN to 30 nN as sliding velocity increased from 1 to 100 m/s Change of friction coefficient wrt contact area and tip shape

Year	Researcher	Simulation condition	Used material	Results
1994[54]	Tupper. and Brenner	* Lennard-Jones potential * Harmonic potential for bond and bending * Sliding between SAM chins	Hexadecanethiol Heneicosanethiol Gold surface	Frictional force between SAM chains increased from 0.001 to 0.008 as normal load increased from 0.05 to 0.6 gf Validity of Amonton's law in nano-scale
2004[55]	Lan and Zhang	* Lennard-Jones potential * Harmonic potential for bond and bending * EAM potential * Sliding between SAM film	SAM film Gold surface Gold tip	Change of tilt angle of SAM film wrt distance between tip and film Frictional force fluctuated when tilt angle of SAM changed
2002[56]	Zhang and Jiang	* Lennard-Jones potential * Sliding between SAM	Alkyl monolayer Si substrate	Decrease of friction force of hydrophilic surface from 0.5 to 0.2 ashumidity increased from 15 to 80%
2003[57]	Tanaka et al.	* Amber force field * Sliding between PFPE	PFPE Zdol film	Friction coefficient decreased from 0.8 to 0.2with increasing normal load Stick-slip of lubricant
2005[58]	Sung and Kim	* Lennard-Jones potential * Morse potential * Scribing Alkanethiol with Si tip	Alkanethiol Si tip Silver substrate	Change of cutting force wrt scribing velocity Wear of SAM depended on scribing velocity and tip shape

topics were reviewed. Atomic friction models were reported by many researchers to explain the behavior of atoms in nano-scale friction. Theoretical and experimental researches were conducted to understand the effects of variables such as load, speed, temperature, humidity, material, contact area, surface roughness, and texturing on nano-scale tribological phenomena. Table 1 summarizes the results of nano-friction research conducted by numerous researchers. Based on the results of these works, there were a few major characteristics that differentiated nano-frictional behavior to that of macro-scale friction. For instance, stick-slip behavior was prominent in atomic-scale frictional interaction and the frictional force was often found to be dependent on the sliding velocity. Though the friction coefficient values varied significantly depending on the experimental condition, in many cases the value was reported to be below 0.1.

As for the analytical approach to investigating nano-friction MD simulation techniques have been effectively utilized. MD analysis is useful in that atomic-scale phenomena that are difficult to investigate experimentally may be simulated numerically. However, due to limited number of atoms that can be modeled and insufficient availability of material potential functions MD simulations have been performed on relatively simple tribological systems. Nevertheless it provides useful insight for the behavior of atoms during nano-frictional interaction. Table 2 summarizes the results of numerous works on numerical analyses of nano-friction.

As can be noted from the results summarized in Tables 1 and 2 extensive research has been conducted on the topic of nano-friction, However, a unified and clear understanding behind the mechanism of nano-scale friction is yet to be achieved. Given the importance of this topic, driven by the development of nanotechnology, the need for continued research effort in nano-tribology remains. With the development of more sophisticated surface analysis tools the objective to control friction and wear is expected to achievable in the future.

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REFERENCES

1. Stachowiak, G. W. and Batchelor, A. W., “Engineering tribology,” Butterworth-Heinemann, pp. 1-9, 2000.
2. Bhushan, B., “Principles and applications of tribology,” John Wiley & Sons, Inc, 1999.
3. Jost, H. P., “Tribology - origin and future,” Wear, Vol. 136, No. 1, pp. 1-17, 1990.
4. Meyer, E., Overney, R. M., Dransfeld, K. and Gyalog, T., “Nanoscience: friction and rheology on the nanometer scale,” World Scientific, pp. 1-28, 2002.
5. Suh, N. P., “The Genesis of Friction,” Wear, Vol. 69, No. 1, pp. 91-114, 1981.
6. VenKatachalam, S. and Liang, S. Y., “Effects of ploughing forces and friction coefficient in microscale machining,” J. Manuf. Sci. Eng., Vol. 12, No. 2, pp. 274-280, 2007.
7. Liu, Z., Sun, J. and Shen, W., “Study of plowing and friction at the surfaces of plastic deformed metals,” Tribol. Int., Vol. 35, No. 8, pp. 511-522, 2002.

8. Houston, J. E. and Kim, H. I., "Adhesion, friction, and mechanical properties of functionalized alkanethiol self-assembled monolayers," Acc. Chem. Res., Vol. 35, No. 7, pp. 547-553, 2002.
9. Tambe, N. S. and Bhushan, B., "Scale dependence of micro/nano-friction and adhesion of MEMS/NEMS materials, coatings and lubricants," Nanotechnology, Vol. 15, No. 11, pp. 1561-1570, 2004.
10. Sung, I.-H., Lee, H.-S. and Kim, D.-E., "Effect of surface topography on the frictional behavior at the micro/nano-scale," Wear, Vol. 254, No. 10, pp. 1019-1031, 2003.
11. Bhushan, B., "Nanotribology and nanomechanics of MEMS/NEMS and BioMEMS/BioNEMS materials and devices," Microelectron. Eng., Vol. 84, Issue 3, pp. 387-412, 2007.
12. Fan, L.-S., Tai, Y.-C. and Muller, R. S., "Integrated Movable Micromechanical Structures for Sensors and Actuators," IEEE Trans. Electron Devices, Vol. 15, No. 6, pp. 724-730, 1988.
13. McFadyen, I. R., Fullerton, E. E. and Carey, M. J., "State-of-the-art magnetic hard disk drives," MRS Bull., Vol. 31, pp. 379-383, 2006.
14. Wang, R.-H. and Nayak, U. V., "Head-disk interface considerations at 10-nm flying height," IEEE Trans. Magn., Vol. 38, No. 2, pp. 2132-2134, 2002.
15. Lee, S.-C. and Polycarpou, A. A., "Effect of hard-disk drive spindle motor vibration on dynamic microwaviness and flying-height modulation," Tribol. Int., Vol. 38, No. 6-7, pp. 665-674, 2005.
16. Kim, D. E., Chung, K. H. and Cha, K. H., "Tribological design methods for minimum surface damage of HDD slider," Tribol. Int., Vol. 36, No. 4-6, pp. 467-473, 2003.
17. Tan, A. H. and Cheng, S. W., "A novel textured design for hard disk tribology improvement," Tribol. Int., Vol. 39, No. 6, pp. 506-511, 2006.
18. Jianbin, L., Shizhu, W., Li, L. K. Y. and Wong, P. L., "Progresses and problems in nano-tribology," Chin. Sci. Bull., Vol. 43, No. 5, pp. 369-378, 1998.
19. Hirano, M., "Atomistics of friction," Surf. Sci. Rep., Vol. 60, Issue 8, pp. 159-201, 2006.
20. Persson, B. N. J., Sivebaek, I. M., Samoilov, V. N., Zhao, K., Volokitin, A. I. and Zhang, Z., "On the origin of Amonton's friction law," J. Phys.: Condens. Matter, Vol. 20, Issue 39, pp. 1-11, 2008.
21. Tomlinson, G. A., "A molecular theory of friction," Philos. Mag. Vol. 7, No. 46, pp. 905- 939, 1929.
22. Dienwiebel, M., Verhoeven, G. S., Pradeep, N. and Frenken, J. W. M., "Superlubricity of Graphite," Phys. Rev. Lett., Vol. 92, No. 12, pp. 126101-1 - 126101-4, 2004.
23. Muser, M. H., "Structural lubricity: Role of dimension and symmetry," Europhys. Lett., Vol. 66, No. 1, pp. 97-103, 2004.
24. Weiss, M. and Elmer, F.-J., "Dry friction in the Frenkel-Kontorova-Tomlinson model: Static properties," Phys. Rev. B, Vol. 53, No. 11, pp. 7539-7549, 1996.
25. Kontorova, T. and Frenkel, Y. I., "On the theory of the plastic deformation and twinning," Zh. Eksp. Teor. Fiz., Vol. 8, pp. 89-95, 1938.
26. Mansfield, M. and Needs, R. J., "Application of the Frenkel-Kontorova model to surface reconstructions," J. Phy.: Condens. Matter, Vol. 2, No. 10, pp. 2361-2374, 1990.
27. Weiss, M. and Elmer, F.-J., "Dry friction in the Frenkel-Kontorova-Tomlinson model: Static properties," Phys. Rev. B, Vol. 53, No. 11, pp. 7539-7549, 1996.
28. Gyalog, T. and Thomas, H., "Friction between atomically flat surfaces," Europhys. Lett., Vol. 37, No. 3, pp. 195-200, 1997.
29. Bowden, F. P. and Tabor, D., "The friction and Lubrication of Solids," Oxford : Clarendon Press, pp. 78-89, 2001.
30. Mate, C. M., McClelland, G. M., Erlandsson, R. and Chiang, S., "Atomic-scale friction of a tungsten tip on a graphite surface," Phys. Rev. Lett., Vol. 59, No. 17, pp. 1942-1945, 1987.
31. Akamine, S., Barrett, R. C. and Quate, C. F., "Improved atomic force microscope images using microcantilevers with sharp tips," Appl. Phys. Lett., Vol. 57, No. 3, pp. 316-318, 1990.
32. Fujisawa, S., Sugawara, Y., Ito, S., Mishima, S., Okada, T. and Morita, S., "The two-dimensional stick-slip phenomenon with atomic resolution," Nanotechnology, Vol. 4, No. 3, pp. 138-142, 1993.
33. Ruan, J.-A. and Bhushan, B., "Frictional behavior of highly oriented pyrolytic graphite," J. Appl. Phys., Vol. 76, No. 12, pp. 8117-8120, 1994.
34. Jiang, Z., Lu, C.-J., Bogy, D. B., Bhatia, C. S. and Miyamoto, T., "Nanotribological characterization of hydrogenated carbon films by scanning probe microscopy," Thin Solid Films, Vol. 258, Issues 1-2, pp. 75-81, 1995.
35. Bhushan, B. and Li, X., "Micromechanical and tribological characterization of doped single-crystal silicon and polysilicon films for microelectromechanical systems devices," J. Mater. Res., Vol. 12, No. 1, pp. 54-63, 1997.
36. Bhushan, B. and Kulkarni, A. V., "Effect of normal load on microscale friction measurements," Thin Solid Films, Vol. 278, Issue 1, pp. 49-56, 1996.
37. Tambe, N. S. and Bhushan, B., "Friction model for the velocity dependence of nanoscale friction," Nanotechnology, Vol. 16, No. 10, pp. 2309-2324, 2005.
38. Bhushan, B. and Sundararajan, S., "Micro/nanoscale friction and wear mechanisms of thin films using atomic force and friction force microscopy," Acta Mater., Vol. 46, No. 11, pp. 3793-3804, 1998.

39. Nair, R. P. and Zou, M., “Surface-nano-texturing by aluminum-induced crystalliuzation of amorphous silicon,” Surf. Coat. Technol., Vol. 203, Issues 5-7, pp. 675-679, 2008.

40. Chung, K.-H., Jang, C.-E. and Kim, D.-E., “Wear characteristics of microscopic bushings for MEMS applications investigated by an AFM,” J. Micromech. Microeng., Vol. 17, No. 9, pp. 1877-1887, 2007.

41. Chung, K.-H., Lee, Y.-H., Kim, Y.-T., Kim, D.-E., Yoo, J. and Hong, S., “Nano-tribological characteristics of PZT thin film investigated by atomic force microscopy,” Surf. Coat. Technol., Vol. 201, Issue 18, pp. 7983-7991, 2007.

42. Chung, K.-H., Kim, H.-J., Lin, L.-Y. and Kim, D.-E., “Tribological characteristics of ZnO nanowires investigated by atomic force microscope,” Appl. Phys. A, Vol. 92, No. 2, pp. 267-274, 2008.

43. Frenkel, D. and Smit, B., “Understanding Molecular Simulation : From Algorithms to Applications,” Academic Press, pp. 63-64, 2001.

44. Friesner, R. A., “Ab initio quantum chemistry : Methodology and applications,” Proc. Natl. Acad. Sci. USA., Vol. 102, No. 19, pp. 6648-6653, 2005.

45. Sham, T.-L. and Tichy, J., “A scheme for hybrid molecular dynamics/finite element analysis of thin film lubrication,” Wear, Vol. 207, No. 1, pp. 100-106, 1997.

46. Kim, D. E. and Suh, N. P., “Molecular Dynamics Investigation of Two-Dimensional Atomic-Scale Friction,” J. Tribol., Vol. 116, No. 2, pp. 225- 231, 1994.

47. Sorensen, M. R., Jacobsen, K. W. and Stoltze, P., “Simulations of atomic-scale sliding friction,” Phys. Rev. B, Vol. 53, No. 4, pp. 2101-2113, 1996.

48. Lia, B., Clapp, P. C., Rifkin, J. A. and Zhang, X. M., “Molecular dynamics simulation of stick-slip,” J. Appl. Phys., Vol. 90, No. 6, pp. 3090-3094, 2001.

49. Belak, J. and Stowers, I. F., “A molecular dynamics model of the orthogonal cutting process,” Proc. ASPE Annu. Conf., pp. 76-79, 1990.

50. Cagin, T., Che, J., Gardos, M. N., Fijany, A. and Goddard, W. A. III, “Simulation and experiments on friction and wear of diamond: a material for MEMS and NEMS application,” Nanotechnology, Vol. 10, No. 3, pp. 278-284, 1999.

51. Komanduri, R., Chandrasekaran, N. and Raff, L. M., “MD simulation of indentation and scratching of single crystal aluminum,” Wear, Vol. 240, No. 1-2, pp. 113-143, 2000.

52. Wu, H., Lin, B., Yu, S. Y. and Zhu, H. T., “Molecular Dynamics Simulation on the Mechanism of Nanometric Machining of Single-crystal Silicon,” Mater. Sci. Forum, Vol. 471-472, pp. 144-148, 2004.

53. Yang, J. and Komvopoulos, K., “A Molecular Dynamics Analysis of Surface Interference and Tip Shape and Size Effects on Atomic-Sclae Friction,” J. Tribol., Vol. 127, Issue 3, pp. 513-521, 2005.

54. Tupper, K. J. and Brenner, D. W., “Molecular dynamics simulations of friction in self-assembled monolayers,” Thin Solid Films, Vol. 253, No. 1-2, pp. 185-189, 1994.

55. Lan, H. and Zhang, S., “Molecular dynamics simulation on nanotribological properties of molecular deposition film during the scan process,” Tribol. Int., Vol. 37, No. 8, pp. 661-665, 2004.

56. Zhang, L. and Jiang, S., “Molecular simulation study of nanoscale friction for alkyl monolayers on Si(111),” J. Chem. Phys., Vol. 117, No. 4, pp. 1804-1811, 2002.

57. Tanaka, K., Kato, T. and Matsumoto, Y., “Molecular Dynamics Simulation of Vibrational Friction Force Due to Molecular Deformation in Confined Lubricant Film,” J. Tribol., Vol. 125, No. 3, pp. 587-591, 2003.

58. Sung, I.-H. and Kim, D.-E., “Molecular dynamics simulation study of the nano-wear characteristics of alkanethiol self-assembled monolayers,” Appl. Phys. A, Vol. 81, No. 1, pp. 109-114, 2005.