

8

Investigation the essence of multibody mechanical attrition of surface at atomic scale

Xuesong Han

School of Mechanical Engineering, Tianjin University, China

Outline:

Introduction.....	217
Basic concepts of atomistic modeling.....	219
Two-body mechanical attrition at atomic scale.....	223
Three-body mechanical attrition at atomic scale.....	233
Conclusion.....	242
References.....	242

Introduction

Mechanical attrition is an important and widely used technique in the area of microelectronic manufacturing and computer manufacturing technology. Many surface machining techniques using mechanical attrition depend upon mechanical processes, which have close relationships with microdynamic behavior of nanoparticles. The complex multibody interactions among nanoparticles and materials surfaces are different from interactions in the macroscopic multibody system, which means that the traditional classical materials machining theory cannot accurately uncover the mystery of the surface generation in the mechanical attrition process. In mechanical attrition, the main objectives are to minimize friction and wear of the abrasive particles whilst maximizing abrasive wear of the workpiece. Other factors that need to be considered are the quality of the workpiece, including the achievement of a specified surface texture and avoidance of thermal damage. Generally, machining of materials surface can be divided into two categories disregarding the interaction among particles, namely, two-body abrasion and three-body abrasion (figure 8.1). In two-body attrition, the abrasive particles are assumed to be constrained by the tool. The relative motion between the particle and the workpiece may be considered to be pure sliding whilst the abrasive grains are free to rotate and slide in three-body abrasion, experiencing collisions both with the workpiece and with the tool and other abrasive grains. The multibody concept is interesting and expected to contribute to the ultimate complete understanding of mechanical attrition processes. The multibody concept is helpful in improving the identification of particulate-related mechanical attrition systems. It implies that each body is a well-defined entity, generally of a single phase. The attrition process can produce new phases, such as wear debris, which become independent bodies and behave according to their own rules. This is generally a one-way sequence of events, and the overall system behavior can be considered by an outside observer to be a chronological sign of the system history. It is inconceivable for the process to spontaneously reverse itself, such as by relocation of the wear particles into their original sites on the worn body.

Mechanical attrition is a complex subject which includes various forms of surface interactions, along with various contacting materials, various demands, and unlimited types of enigmatic failures. The vast

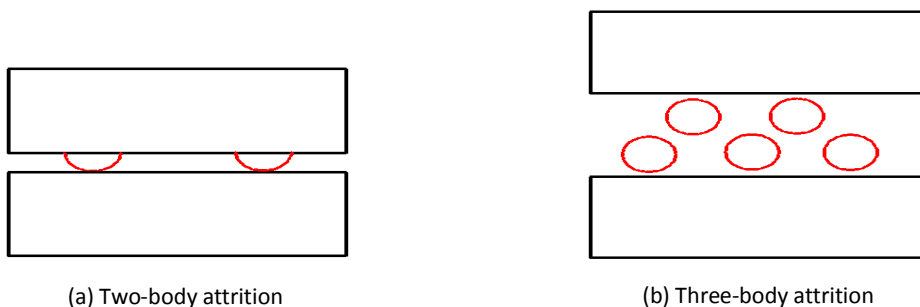


FIGURE 8.1

Different attrition mode

amount of research in the field of mechanical attrition excels in its diversity. The multibody concept makes a gallant attempt to offer a rational guide for planning and executing mechanical attrition research and modelling. The multibody concept is a useful theoretical tool for establishing a relationship between microscopic mechanisms and the macroscopic properties such as wear, friction and load carrying capacity of machining systems. From the point of view of surface degradation, the

wear process under dry rubbing condition is considered as a particle flow including material detachment (by different possible mechanisms such as adhesion, abrasion, fatigue, oxidation) from the first bodies leading to the formation of third body particles with their possible elimination from the contact as wear particles. The multibody which exists or is created in the contact of two rubbing solids often exhibits a granular or particulate structure. This may occur at different levels: it is well known that the generation behavior and evolution of wear debris often plays an essential part in the friction and wear mechanisms. This particulate structure however may also appear at a more microscopic level like for instance in colloidal lubrication where the interaction between colloid particles partially controls the action of the lubricant. From a more fundamental point of view and in opposition with the bulk behavior which can essentially be described at a macroscopic and continuum level, a correct understanding of surface phenomena basically requires a description at the microscopic molecular level which is responsible for such effects as surface energy, capillarity adhesion and so on. The discrete nature of materials and in particular of the multibody must therefore be taken into account. Direct simulation and the corresponding numerical experiments will provide a tool for enhancing the understanding, complementary to the usual macroscopic mechanical analysis.

In most of mechanical attrition process, whether it be metallic, polymeric or ceramic systems, an important and frequent consequence of the action of the sliding motion, between two interacting surfaces, is the formation of an interphase whose properties, chemical and physical, are different to those of the adjacent (or first) bodies: a third body. The physical characteristics of such systems are greatly dependent upon the response of this resultant third body. For example, the steady state attrition is modified and controlled according to the dynamics and properties of the third body that is produced. For elastic and brittle materials, the third body is generally in the form of particulate debris, which may or may not affect the friction process. For more plastic and viscous materials, the sliding motion often gives rise to the formation of a transformed film, the properties of which are generally different from those of the contacting bodies. Such interface films are generally formed from a molten/softened surface layer at the contacting point of the two bodies. In some cases, they are generated also by the presence of a lubricant or humidity in the vicinity of the contact. For instance, the presence of humidity or water can lead to the formation of hydroxides for ceramic systems. These hydroxides act as a third body which may lead to an increase in the wear of the material. Surface melting is a common occurrence in polymeric contacts sliding and this molten layer behaves more or less in a viscous manner. Generally, such interactions are engineered between a coherent rough soft material sliding against a hard substrate. A soft material, for example a polymer sliding against a hard metal, shows localized surface melting at elevated temperatures due to frictional heating and this molten layer facilitates the localized frictional energy dissipation by a viscous flow process. Similarly, isothermal strain softening may occur due to the localized interfacial restructuring or reorientation. A similar observation of a third body formation has also been reported in the different but important area of material processing involving paste deformation and flow. Pastes are an example of soft solids which exhibit comparatively low yield stresses. They are normally constituted from fine particles dispersed in a liquid phase; the solid phase volume fraction is typically 60%. The boundary layer formation in paste flow is the result of the presence of a liquid-rich region near the rigid wall due to the large shearing action between the solid particles present in the paste and the rigid wall. The formation of a "third body" in soft-solid processing is of special significance as this phase, in a large part, controls the efficiency of the processing operations.

Mechanical attrition as a surface machining technique can be divided into two groups, bonded and loose corresponding to two-body and three-body concepts. In the bonded process, the machining operation is accomplished by two main elements while the machining operation is accomplished by three elements in the loose process. In the common bonded mechanical attrition process, an abrasive

tool is used for operations such as grinding, cut-off, honing, and sometimes polishing. The main constituent is an abrasive layer with a composite structure. The abrasive layer is held in a tool holder or attached to a backing. The composite includes the grit within a matrix. The layer is made up of hard abrasive grit and bond material to retain the grit within a tridimensional structure. The grit and the bond have very different physical-mechanical properties. The hardness are of one order of magnitude different. The main contact between the tool surface and the workpiece takes place on the hard and sharp edges of the grit. The hardness of the grit is sufficient to plastically deform the workpiece material, as required in ploughing and cutting the workpiece surface. The deformations of the abrasive particles are negligible compared with deflections of the bond. The elastic properties of the tool itself are favorable for finishing and super-finishing actions, and are achieved by an appropriate choice of the type, hardness, and structure of the bond. The technology of manufacturing abrasive composites and their application in the processing of different materials represent the result of extensive studies on the process of abrasive wear. The emergence of synthetic composites can be justified by the very high values of the abrasive-wear intensities achieved, in comparison with the other three basic wear mechanisms. In abrasive machining, the aim is to achieve a wear process on the workpiece while minimizing wear on the tool. Irrespective of whether abrasive wear is considered to be a benefit or a disadvantage, the lessons from tribology can be usefully applied to develop and utilize abrasive tools. The loose mechanical attrition process which belongs to a family of fine-finishing processes generally consists of a workpiece and a supporting element, i.e., a lap or a polishing pad, with a low or medium hardness to pressurize the loose abrasive grains against the workpiece. The supporting abrasive element may be supplied by means of a fluid suspension to transport the grits. The fluid suspension also lubricates and cools the machining process. In fine-finishing operations, swarf must be removed by washing debris from the processed surface. The fluid used for the processing and washing are often evacuated from the system, together with the swarf, without recycling.

Interaction between nanoparticle and solid surface are of fundamental importance to science and technology. The appearance of macroscopic particle-surface interactions is well known from experiences in daily life. As the size of the particles decreases and approaches molecular dimensions, their atomic nature becomes increasingly important. Interactions on the molecular level can be studied experimentally using molecular beam techniques, and theoretically by molecular dynamics simulations. In the current research, MD simulations are used to study the interactions between nanoparticle and substrate. Nanoparticles are relatively large and behave as “macroscopic” particles in some respects. At the same time they are small enough to permit the long-time simulations necessary for investigation of self-organization processes. Interactions between nanoparticles and surfaces have been studied for over a decade due to their relevance for both fundamental and applied research. A variety of processes may occur depend on the properties of the nanoparticle, the available energy and the energy transfer rates involved. A straightforward interpretation of experimental results is often not possible due to the complexity of the dynamics. Atomistic modeling provide an efficient method for studying the details about the dynamic behavior of atom/molecule/particle at small scale which is helpful about understanding physical essence of mechanical attrition.

Basic concepts of atomistic modeling

Over the last decades, there has been a new realization that understanding the nanoscale behavior is required for understanding how materials removal/deformation. Molecular dynamics simulation is a numerical technique for computing the equilibrium and transport properties of classical many-particle system which can provide a fundamental description of the materials fracture (removal) and

deformation happened at atomic level. Generally speaking, molecular dynamics is a model based microscopic description of real physical system. The system can be few- or many-body system. The description may be a Hamiltonian or, Lagrangian or expressed directly in Newton equations of motion. The molecular dynamics method calculates properties using the equation of motion and obtains the static as well as the dynamic properties of system. The essence of the MD simulation method is the numerical solution of Newton's equation of motion for an ensemble of atoms. These equations are integrated by numerical techniques for extremely short time intervals (2-3fs), and equilibrium statistical averages are computed as temporal averages over the observation time. In principle, explicit knowledge of the electronic ground state in each system configuration is required in order to have a correct description of the interatomic forces. To render atomistic simulation studies practical, a classical or semi-classical potential from which interatomic forces can be derived is necessary. This is accomplished by using an appropriate empirical potential energy function that satisfies stringent material properties criteria that include the lattice constant, energy of sublimation, compressibility, elastic constants, the equation of state and the stability of the crystal itself. Experiments are generally performed on a macroscopic sample which contains a larger number of atoms or molecules sampling an enormous number of conformations. In statistical mechanics, averages corresponding to experimentally measured values are defined in terms of ensemble averages. An ensemble average is an average take over a large number of replicas of the system considered simultaneously. In MD simulations, the points in the ensemble are calculated sequentially in time, so in order to calculate the ensemble average, the MD simulation must pass through all possible states corresponding to the particular thermodynamic constraints. In reality, the MD simulation calculates the time average while experimental results correspond to ensemble average. The problem is solved by the assumption that the time average is equal to the ensemble average.

The fundamental mathematical problem considered throughout this chapter is a non-continuum problem called the N-body problem, which is described in complete generality as follows. In cgs units and for $i = 1, 2, \dots, N$, let P_i of mass m_i be at $\vec{r}_i = (x_i, y_i, z_i)$, have velocity $\vec{v}_i = (v_{i,x}, v_{i,y}, v_{i,z})$, and have acceleration $\vec{a}_i = (a_{i,x}, a_{i,y}, a_{i,z})$ at time $t \geq 0$. Let the positive distance between P_i and P_j , $i \neq j$, be $r_{ij} \neq r_{ji} \neq 0$. Let the force on P_i due to P_j be $\vec{F}_{ij} = \vec{F}_{ij}(r_{ij})$, so that the force depends only on the distance between P_i and P_j . Also, assume that the force \vec{F}_{ij} on P_j due to P_i satisfies $\vec{F}_{ij} = -\vec{F}_{ji}$. Then, given the initial positions and velocities of all the P_i , $i = 1, 2, 3, \dots, N$, the general N-body problem is to determine the motion of the system if each P_i interacts with all the other P_j 's in the system.

Statistical Ensembles

Molecular dynamics simulation is a theoretical toolkit of studying the natural time evolution of classical system composed of N particles in volume V and converse this very detailed information into macroscopic terms. There is a need to understand the way in which the relatively complicated microscopic many-body dynamics gives rise to the relatively simple macroscopic few-variable behavior described by phenomenological thermodynamics and hydrodynamics. The thermodynamic state of small scale system is usually defined by a set of parameters (such as the number of particles N , the temperature T and the pressure P). Although there are still many other thermodynamic quantities, all of them can be derived through knowledge of the equations of state and the fundamental equations of thermodynamics. While most of these parameters convey some properties about the microscopic structure and dynamics of the system, their values are completely dictated by the few variables (such as NPT) characterizing the thermodynamic state but not by the very many atomic positions and

momenta that define the instantaneous mechanical state. Some of the variables useful for describing macroscopic systems have obvious microscopic analogs. The macroscopic mass ρdr and the momentum $\rho v dr$ in a volume element dr , for instance, correspond to simple sums of one-particle contributions. The macroscopic energy and the pressure tensor are more complicated functions. They include not only one-particle kinetic part, but also two- or more-particle potential contributions. Molecular simulations permit the rigorous application of the principles of statistical mechanics to calculate the properties of a chosen system. From the viewpoints of statistical mechanics, a system's macroscopic properties such as pressure or density represent averages over all possible quantum states. To calculate the properties of real system, it is convenient to define an ensemble. An ensemble can be regarded as an imaginary collection of a very large number of systems in different quantum states with common macroscopic attributes. For example, each system of the ensemble must have the same temperature, pressure and the number of molecules as the real system it represents. The ensemble average of any property $\langle A \rangle$ can be obtained from the relationship:

$$\langle A \rangle = \sum_{i=1}^n A_i p_i \quad (\text{x.1})$$

here A_i is the value of A in quantum state i , p_i represents the probability of observing the i th state, and the angled brackets denote an ensemble average. The time-averaged properties of the real system are related to the ensemble average as stated in the previous section. The equivalence of the time-average and the ensemble-average is called the ergodic hypothesis. The form of p_i is determined by which macroscopic properties are common to all of the systems of the ensemble.

Numerical Methodology

It will be necessary in molecular modeling to solve the system of second order differential equations from given initial data. Since, in general, F will be nonlinear, numerical methodology will be essential. Our choice of numerical methods will be guided by the following two observations. First, since ϕ depends only on r , the system is completely conservative, that is, the system's energy, linear momentum, and angular momentum are time invariants. Second, for many potentials and forces to be considered, $r = 0$ will be a singularity in the sense that the potential or the magnitude of the force becomes unbounded as r goes to zero. For such cases the time step must be small for values of r close to zero, which precludes the basic value of high order numerical techniques.

Molecular simulations aim to predict atom trajectory in the materials include the atomic position, velocity and acceleration. As for thermodynamic ensemble NVE with constant particle number, the volume of system and the total energy of system, the atomistic positions can be acquired by integrated the following equations:

$$r_i(t + \Delta t) = r_i(t) + v_i(t)\Delta t + \frac{F_i(t)}{2m} \Delta t^2 \quad (\text{x.2})$$

$$v_i(t + \Delta t) = v_i(t) + \frac{(F_i(t) + F_i(t + \Delta t))}{2m} \Delta t \quad (\text{x.3})$$

here $F_i(t + \Delta t)$, $v_i(t + \Delta t)$ and $r_i(t + \Delta t)$ are force, velocity and position of the i th atom at the moment $t + \Delta t$ while $F_i(t)$, $v_i(t)$, v_i^n and $r_i(t)$ are force, velocity and position of the i th atom at the moment t , Δt is timestep, m is mass of atom. Other thermodynamic ensembles such as NVT or NPT ensembles can be realized by modifying the equations of motion in an appropriate way.

Potential Function

Whenever a problem is considered at an atomic scale, there is a need to consider the forces that exist between the molecules (atoms), for it is these forces that decide much of what happens in any phenomenon. Intermolecular forces can be loosely classified into various categories. One may divide them into categories of “opposites”-in other words, attractive or repulsive, short-ranged or long-ranged, strong or weak, and isotropic or directional. These are important distinctions, but they are also ambiguous and confusing. A force that has the same physical origin may be both short-ranged and long-ranged, or it may be attractive in one solvent and repulsive in another. This way of classification can also result in the same force being “counted twice” in any theoretical analysis. To avoid such pitfalls, it is best to classify forces according to their different physical or chemical origin, although even here we shall see that the forces among large particles or extended surfaces lend themselves to different modes of classification from those occurring between two atoms or molecules; this is because of the collective interaction among many molecules, which always includes entropic effects and cannot be easily related to the individual pair potentials.

A potential that is developed for one class of material in all likelihood would not be satisfactory for application to other classes of materials, because the interacting forces are so different. It is therefore necessary to develop a potential for each class of material. Unfortunately, the development of a potential is not a simple, straightforward approach and may take considerable time and expertise. Fortunately, potentials were developed for limited classes of materials and research is in progress for other materials. For example, Morse and Lennard-Jones potentials were applied initially to address cubic metals. Embedded atom potential was developed as an improvement for a wider range of metals. Similarly, Brenner potential and Tersoff potential were developed to address covalently bonded materials, such as silicon, germanium and even diamond. The Born-Meyer potential was developed specifically for some ceramics. It should, however, be noted that these potentials were developed for single-phase, single-crystal materials that have one specific form of bonding. For polycrystalline materials, metallic alloys and for materials which are part ionic and part covalent, the development of new and more complex potentials is required.

The accuracy of the trajectories of atoms obtained from the MD simulation is highly affected by the choice of the appropriate potential energy (PE) function. Hence, selection of an appropriate PE function is a prerequisite. The total energy of a system is the sum of kinetic energy and potential energy. The kinetic energy is simple to compute while the computation of PE is rather complex as it depends on the position of all interacting atoms. The potential energy plays a central role in MD simulation. Firstly, the force acting on each atom is proportional to the first derivative of the PE function. Secondly, the total energy must be carefully monitored in MD simulation. There are two approaches for the determination of interatomic potentials. The first approach is an ab initio method and the second approach uses essentially empirical potentials. In the ab initio method, the parameters of the PE function can, in theory, be determined by solving Schrodinger’s wave equation. However, in practice, it is difficult to solve by this method except for very simple systems. The term “empirical” in empirical potential may be somewhat misleading or oversimplifying as it may not be strictly as empirical as the term suggests. In fact, these potentials often present a more realistic view of the atomic interactions than potentials

derived exclusively at great efforts from purely theoretical considerations which are themselves often approximate in nature. The empirical potentials are based on simple mathematical expressions for the pairwise interaction between two atoms or ions, which may or may not be justified from theory, and which will contain one or more parameters adjusted to the experimental data. The validity of the function as well as the stability of the crystal for a given material are checked for various properties including cohesive energy, the Debye temperature, the lattice constant, the compressibility and the elastic constants as well as the equation of state. Consequently, these potentials can be considered as reasonably valid for simple cubic metals. For larger systems, empirical PE functions are used that take into account factors such as covalent bond stretching and bond angle change due to bending, torsion and non-bonded (van der Waals and Coulomb) interactions. This is the second and most common method in which the parameters are determined on the basis of the physical properties of each material. The parameters can be obtained either from experimental studies or using quantum mechanical calculations. The interatomic potential energy is usually assumed to be the sum of n-body (empirical) potentials which depend only on the distance between the atoms. These potentials are further classified into two-body, three-body and multi-body potentials according to the unit of atoms on which the potential terms depend. The attractive force binds the atoms together while the repulsive force prevents them from coalescing. The magnitude of both forces increases as the distance between them decreases, the repulsive force increasing more rapidly than the attractive force. The curvature of the potential energy function is determined mainly by the repulsive force, which therefore dictates the elastic behavior of the solid. The length of the bond is the center-to-center distance of the bonding atoms. Strong bonds pull the atoms closer and so have smaller bond lengths compared with weak bonds. At some definite distance, the attractive and the repulsive forces exactly balance and the net force is zero. This corresponds to stable equilibrium with a minimum potential energy, the magnitude of which is the bond energy. The cohesive properties of the solid, its melting and vaporization behavior are determined by the magnitude of the maximum binding energy, which is governed by the attractive component of the interatomic force. The PE functions generally extend over a modest range of pair separations though at vanishingly small energy levels. By neglecting the interatomic interactions beyond a cut-off point, a significant reduction in the computational time with minor loss in accuracy can be accomplished. Truncation of the potential to a cut-off point also results in a similar truncation in the force curve. The cut-off distance can be of any value of choice but is generally taken as the distance where the value of the potential energy is about 3-5 percent of the equilibrium potential energy.

Two-body mechanical attrition at atomic scale

During two-body attrition process, the abrasive particles are dragged across the surface and act as cutting tools. Removal volumes are determined by abrasive particle loading and film properties and the removal rates are governed by velocity and particle loading. In industrial applications, the abrasive grit may be bonded to a paper, fabric, or metal surface with a water-soluble or water-resistant adhesive. The grit is spaced in a controlled manner and is often deposited electrostatically to align its sharp edges perpendicular to the backing surface.

The atomic configuration of the system studied is illustrated in figure 8.2. Silicon atoms of slurry particle and substrate are initially arranged in diamond cubic structure with a constant lattice parameter of 5.43 Å. The dimension of silicon workpiece is $180 \times 55 \times 50 \text{ \AA}^3$ along X, Y and Z directions. The moving speed is 20 m/s, the environment temperature is 293 K, the depth of cut is 8 Å, the particle diameter is 16 Å, the timestep is $2.5 \times 10^{-15} \text{ s}$.

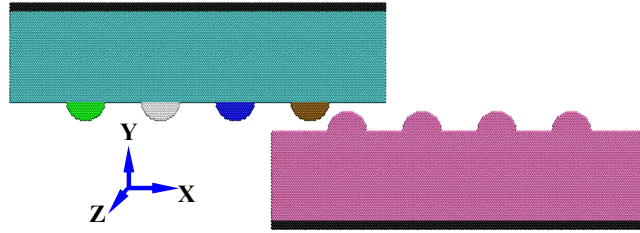


FIGURE 8.2

Atomic configuration of system
ochre: particle1, blue: particle2, white: particle3, lime: particle4

For covalent systems, the Tersoff potential is used to depict the interaction between the substrate atoms and atoms of the abrasive particle as follows:

$$\phi_{ij} = f_c(r_{ij})[f_R(r_{ij}) + b_{ij}f_A(r_{ij})] \tag{x.4}$$

With equation (x.4), the interaction force between silicon atoms can be obtained by calculating the negative gradient of ϕ .

The computation of atom trajectory requires numerical integration of the differential equations from initial state which the abrasive particle is approaching the wafer but has not touched yet to the final state which a layer of material has been removed from the wafer. There is variety of methods available for performing this numerical integration such as fourth-order Runge-Kutta method, Leap-Frog method, Verlet method, Velocity-Verlet method and so on. The Velocity-Verlet method is a symplectic algorithm which can prevent the energy dissipation and have high computation efficiency, this paper adopted this method as follows:

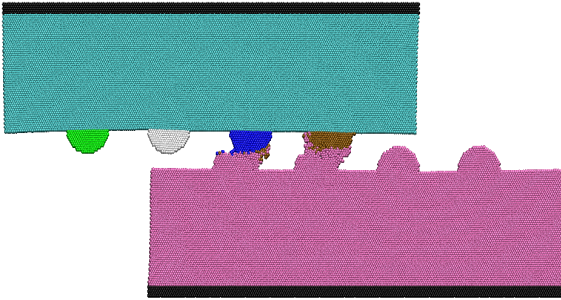
$$r_i^{n+1} = r_i^n + hv^n + \frac{h^2}{2m} F_i^n \tag{x.5}$$

$$v_i^{n+1} = v_i^n + h(F_i^n + F_i^{n+1}) / 2m \tag{x.6}$$

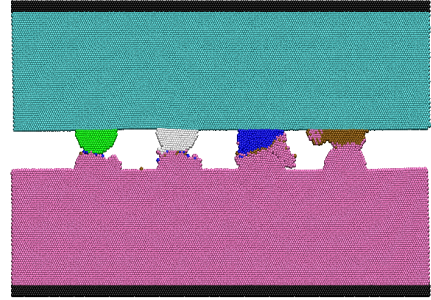
here r_i^{n+1} , v_i^{n+1} and F_i^{n+1} are position, velocity and force at $n+1$ step of the i th atom while r_i^n , v_i^n and F_i^n are position, velocity and force at n step of the i th atom, h is timestep, m is mass of atom.

Wear is the basis of planarization which can fabricate parts with highly controlled shapes and surface finishes. The idea that material is cleanly cut away from the workpiece is preferred to material being rubbed away. However, cutting and rubbing are merely two aspects of attrition whose main objective is more likely to maximize removal rate.

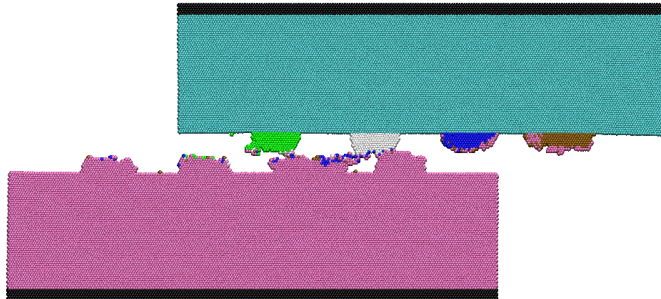
Mechanisms of two-body abrasion on the atomic scale



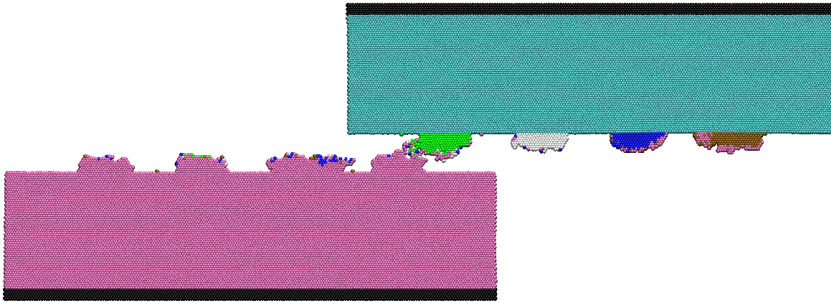
(a) Time step: 28000



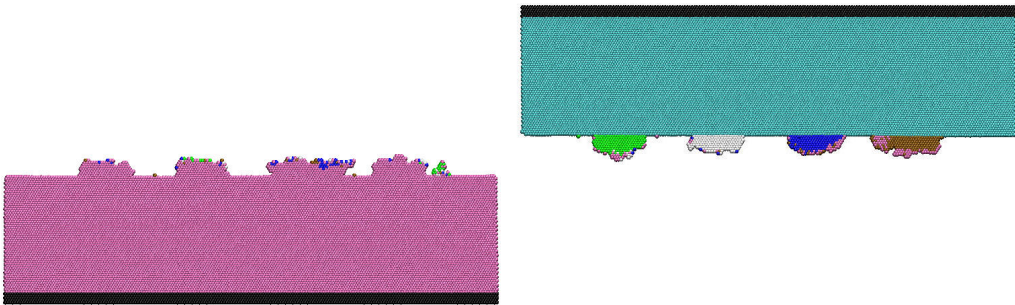
(b) Time step: 56000



(c) Time step: 84000

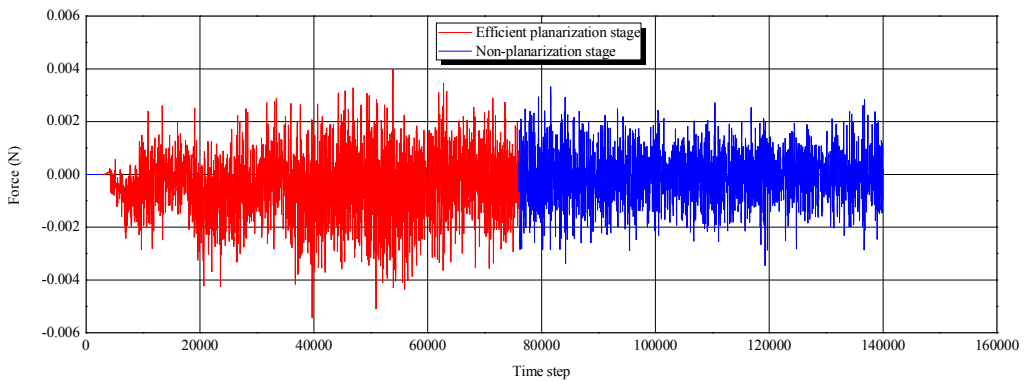


(d) Time step: 112000

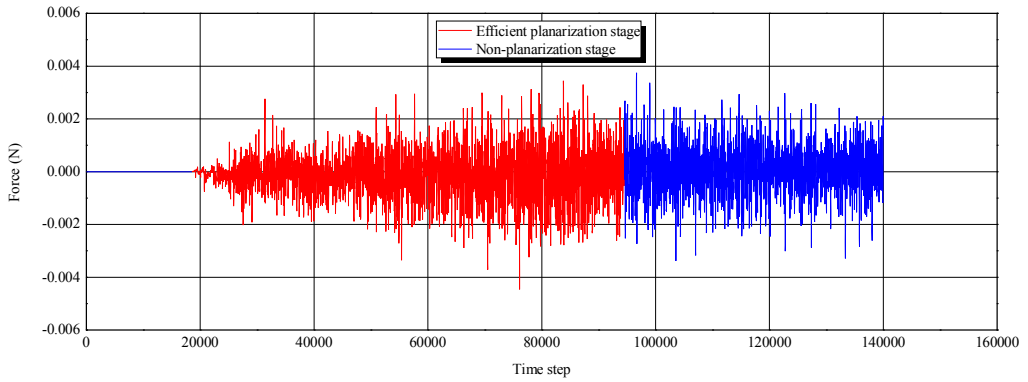


(e) Time step: 140000

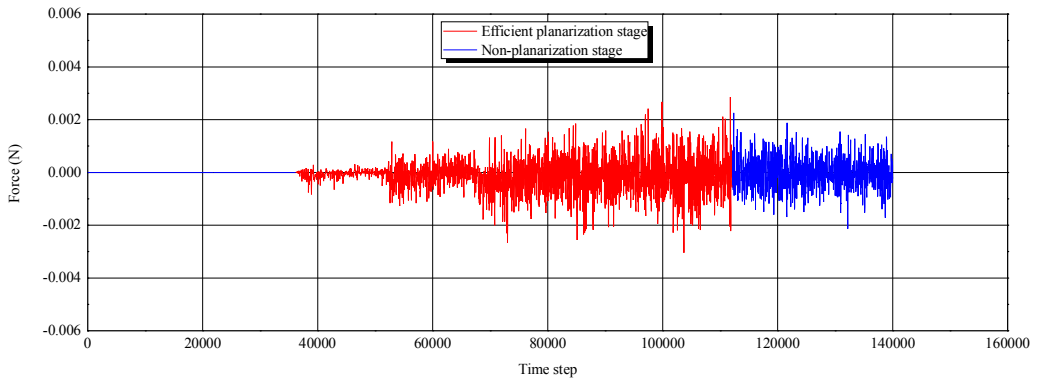
FIGURE 8.3
MD simulation of two-body wear process



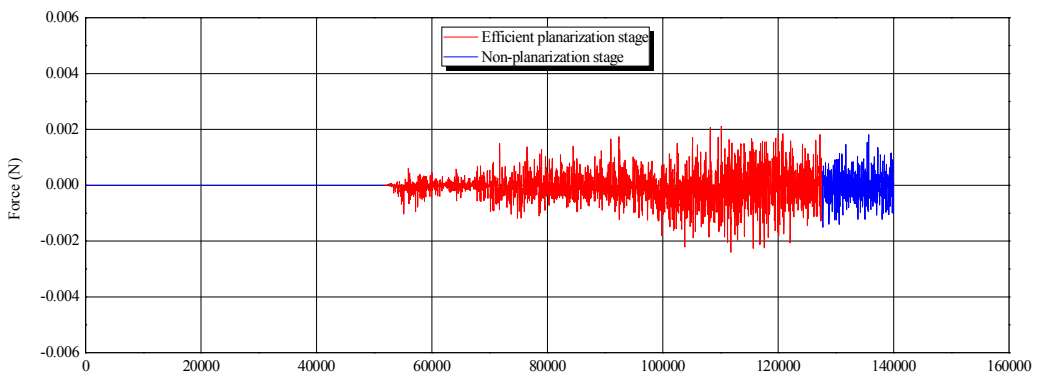
(a) The friction force generated by particle1



(b) The friction force generated by particle2



(c) The friction force generated by particle3



(d) The friction force generated by particle4

FIGURE 8.4
The variation of friction force in the CMP

Figure 8.3~4 shows the MD simulation results of two-body mechanical attrition process at atomic scale. As the two materials approach each other, part of the surface atoms of one material will “touch” the surface atoms of the other material, while in other regions, the surface atoms are separated by larger distance. This tribology behavior leads to the loss of materials from both of the contacting surfaces when subjected to relative motion. In this process, the particles are embedded into the pad which makes them working in a similar conditions as the traditional abrasive machining process such as grinding, honing and so on. In this case, pressure is applied on the abrasive through a conformable pad or soft cloth. This allows the abrasive to follow the contours of the workpiece surface and limits the penetration of individual grains into the surface. Attrition with a fine grit is a very gentle abrasive action between the grains and the workpiece, thus ensuring a very small scratch depth. The scientific principles underlying abrasive machining processes lie within the domain of tribology as wear is the basis of the most abrasive manufacturing processes. Researchers have already provide common mechanisms contributing to this case, namely, the classical model for sliding wear which brought forward by *Archard* and usually referred to as the *Archard wear equation*. This model derives an expression for the wear rate W , which is defined to be the volume V of material removed per unit sliding distance s :

$$W = \frac{V}{s} \quad (\text{x.7})$$

So, a basic assumption of this wear model is that the wear volume is proportional to the sliding distance. While this is generally borne out in experiments, it should be kept in mind that it is not universally true, as wear can change the nature of sliding surfaces to such an extent that the wear mechanism changes. For example, when materials first rub against each other, a running-in or breaking-in period often occurs where the initial wear rate is higher or lower while the surfaces are evolving to their “steady state” of wear.

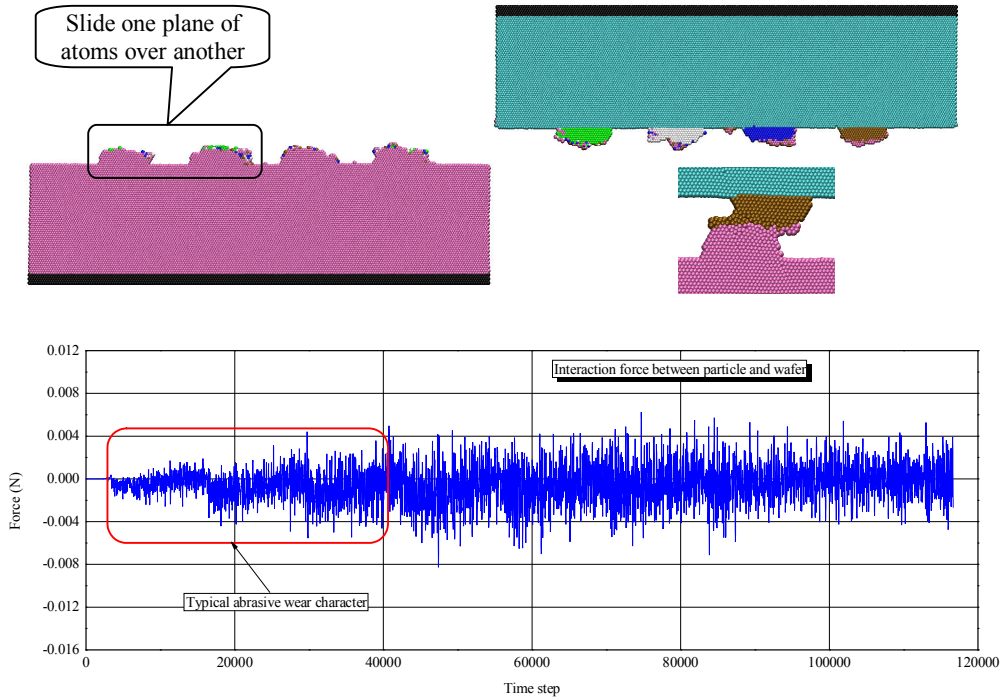
Figure 8.4 shows the variation tendency of friction force induced by different slurry particles. Obvious character is observed about the interaction between particle1 and the first two peaks of the substrate (before 40000 timesteps). After that the particle1 became intensely worn and the friction force gradually tends to be non-typical after it leaves the substrate. The different force variation tendency in figure 8.4 (a) justifies that more than one control mechanism dominate the tribology behavior in the single impact. The planarization effect induced by the particles is gradually weakened because of the wear of the slurry particles. Comparing with particle1, the friction force induced by the other three particles gradually increasing at the initial stage which justifies the final planarization surface is the synergetic behavior of all particles.

Another classical assumption of sliding friction is that, due to surface roughness, contact only occurs where the asperities touch, so the true contact area is the sum of all the individual asperity contact areas. As there are relative lateral motion between the particles and the substrate, the contact area is also closely related to their relative position. The periodically changing of contact spot is observed in the grinding process. Initially, the contact spot is gradually increased and the true contact area is increased accordingly. The contact area approaches the maximum value as the couple materials being aligned completely, after that the true contact area decreased gradually. This phenomenon illuminates that the real contact area is not entirely depended on the external pressure and the multibody interaction is more reasonable for the description of whole working conditions at nanometer scale. Comparing with the fluid-based wear process, this solid-based wear process can generate global planarization surface more efficiently because the semi-rigid constrain (exerting by polishing pad) counterpart the reaction force induced by the substrate. Little plastic deformation extends into the

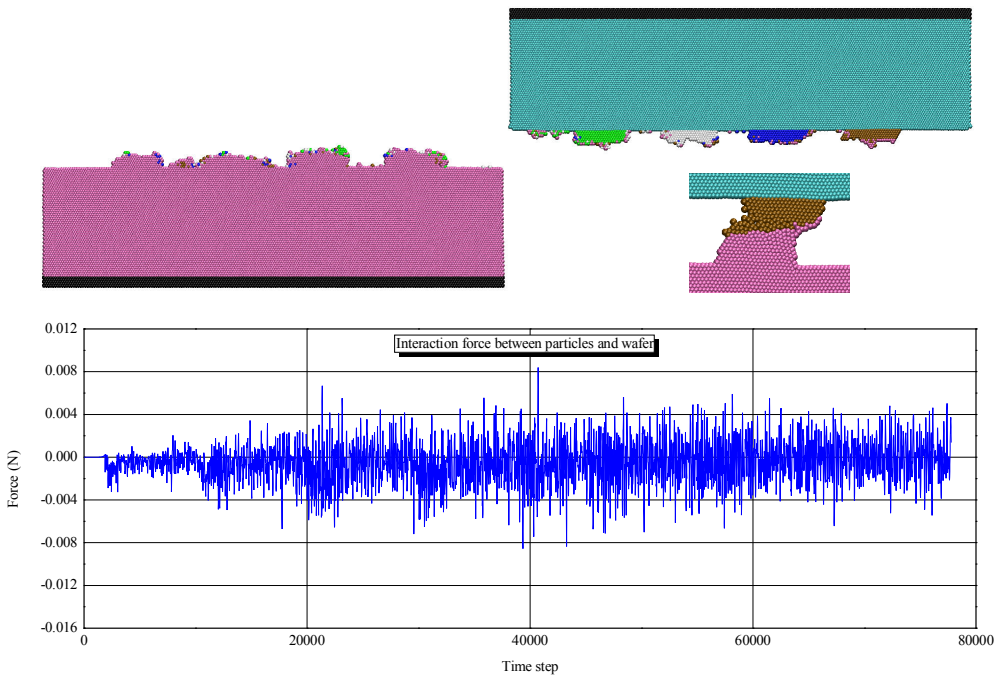
bulk materials far from the local contact area. It is also shown that no dislocation generated in the wafer which means there may be some different control mechanism dominates the wear process at this small length scale. Macro-scale plastic deformation within crystalline materials occurs mainly through the motion of flaws and defects in the crystal structure, called dislocations. When the size of the region undergoing plastic flow becomes much smaller than the typical distance between dislocations, however, the contribution of dislocations to the yield stress becomes insignificant; instead, the yield stress is governed by the force needed to slide one plane of atoms over another. There are obvious different variation trend about the polishing force induced by the four particles. Firstly, the attractive force is induced as the particles approaching the substrate, after that the repulsive force gradually increased and many wafer atoms (atom clusters) are rubbed away. The abrasive particles are gradually worn with the ongoing of the attrition process which decreases the micro-cutting effect and result in different trend of machining force. After that the interaction force tends to be steady. As the abrasive particles slide relative to the wafer surface, the atomic groups experience three stages, namely, interlock, elastic-plastic deformation and finally slip process. The surface planarization is mainly accomplished in the last two stages. Materials removal or plastic deformation induced by two-body tribology behavior is realized near contact spots characterized by high normal and tangential stresses. It can occur due to single or repeated loading of contact spots.

Dynamic evolution of the attrition process at an atomic scale

The atomic and molecular forces combine will dominate the forces acting between solid surfaces. Tribology behavior must originate from the forces between the atoms; so, the various forces act between pairs of atoms and the ways that we can sum up these forces is crucial to the net force in the attrition which acting between surfaces. The mechanical (wear) properties of material originate from how the individual atoms are bond to their neighboring atoms in the material. When two similar atoms are brought together, a bond will form between them. An attractive force, which gradually decreases in magnitude over a range of 4 to 5 atomic diameters as the atoms move apart; a repulsive force, which increases rapidly as the atoms are squeezed together due to the overlap of the electron clouds that surround each atom; and the resultant force, which is the sum of the attractive and repulsive force. For small applied forces, the atoms only move a small fraction of the bond length away from the equilibrium separation distance, and the restoring force is proportional to the distance moved which is termed as elastic deformation. For elastic deformation, the atoms return their original positions if the applied force is removed. If a large enough tensile force is applied to the solid that the force on individual atoms exceeds the critical value, the attractive restoring force will be insufficient to hold the material together and the plastic deformation takes place and many atoms are no longer at their original positions when the applied force is removed.



(a) Velocity: 30 m/s



(b) Velocity: 60 m/s

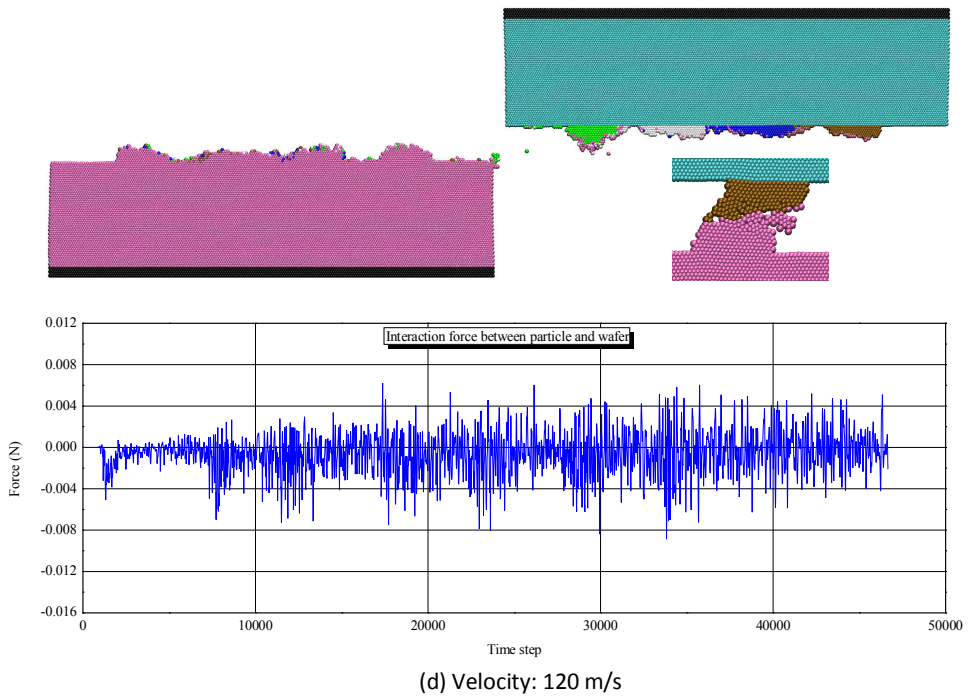
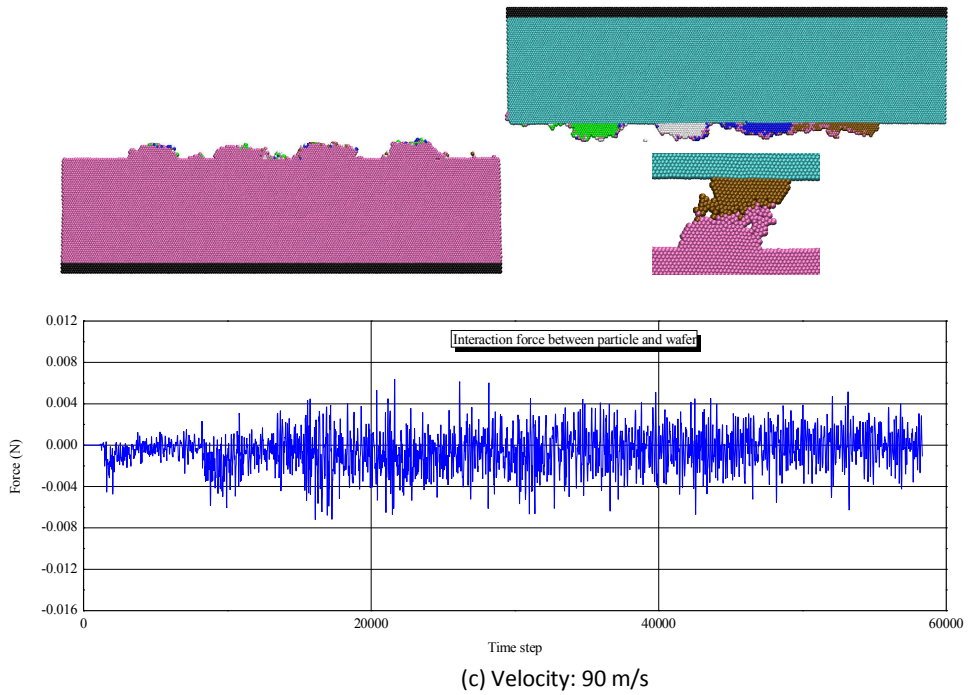
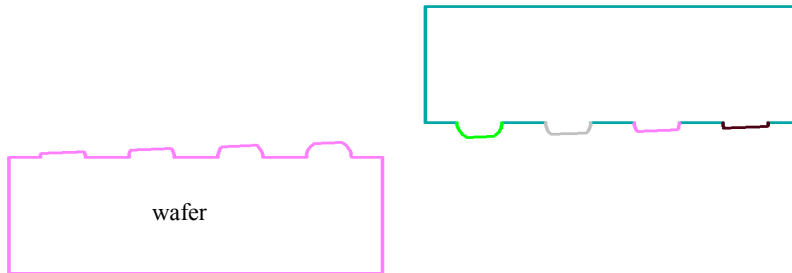


FIGURE 8.5
MD simulation CMP at different velocity

**FIGURE 8.6**

Nominal surface morphology model under abrasive wear dominant mode

Plastic deformation can take place several ways, for brittle materials at macroscopic scale, the atoms do not slide easily past each other. So, when an externally applied tensile force exceeds the attractive force holding the atoms together in the solid, the material just snaps. Many of the wear processes described above involve plastic deformation of material in small localized regions where asperities of the opposing surfaces or hard particles make contact. It turns out that the onset of plasticity for such small regions can be dramatically different than the plastic yield stress determined by macroscopic measurements. In this atomic sliding wear process, atoms slide one atomic position along a slip plane. This slip motion repeats many times along a large number of slip planes and grain boundaries in the solid until all the forces on individual atoms are below the threshold value needed to initiate plastic deformation. In fact, abrasive wear on the atomic scale is the result of the energy barrier that must be overcome to jump over the atomic corrugations on the sample surface. As the particle scratches substrate surface, the interaction force gradually increases until it can overcome the energy (potential) barrier. After some motion, there is enough energy stored in the spring which leads to slip into the neighboring stable equilibrium position and result in typical abrasive wear character (shown in figure 8.5 (a) the rectangle square). Figure 8.5 shows the two-body mechanical attrition process at different sliding speed. The snapped image of the impact between particle1 and the left surface peak (single peak contact) is embedded at right corner of every figure. As for individual asperity contact at this nanoscale, non-obvious Archard adhesive wear character is observed. In Archard's original model, wear occurs when a fragment of material detaches from an asperity during contact. The volume of this fragment is presumed to be proportional to the cube of the contact dimension while the shape of this wear fragment is assumed to be a hemisphere with radius a . Still, this sliding wear does not belong to classical abrasive wear as no obvious abrasive wear character (figure 8.6) is observed. The materials removal mainly limited at the local individual asperity even at high sliding speed.

The interaction between particle and individual asperity of the substrate is strengthened with the increasing of sliding speed as a quickly increasing of interaction force at the initial stage as shown in the figure 8.5. The materials removal mechanism gradually transform from adhesive abrasion to abrasive abrasion. This adhesive abrasion based materials removal is realized through tearing while the abrasive abrasion is accomplished by micro-cutting. Little plastic deformation is generated (such as dislocation) in the whole tribology process. Also the typical brittle crack is not observed in the bulk materials even at the high impact velocity. This traditional brittle material exhibits novel plastic deformation feature in

the nanometer scale tribology-behavior based interaction. The surface planarization and the materials removal efficiency are improved with the increasing of sliding speed. The materials removal process during the engagement of an abrasive cutting edge on the surface of workpiece mainly depends on the physical properties between the active partners. In fact, the simultaneous impact of several abrasive particles or the repeated impact of one abrasive particle leads to material failure at the border of the traces. The results justify that for most sliding systems, no single wear mechanism dominates at all operating conditions; rather, different wear mechanisms operate, with their relative importance changing as the sliding conditions change (surface integrity and the wear of the slurry particles), and with abrupt changes in wear rates occurring when one dominant wear mechanism replaces another. Two-body abrasive process is one of the most important basis of surface planarization which can fabricate parts with highly controlled shapes and nanometer dimensional tolerances with only a few angstroms of roughness. The final nanometer level planarized surface should be the synergetic behavior of slurry particles with different size and different track. Furthermore, new abrasives from other different area will continuously enter the local area. All of the above conditions will be improved and carried out in the following work.

Three-body mechanical attrition at atomic scale

MicroDynamic behavior of particles with zero impact angle

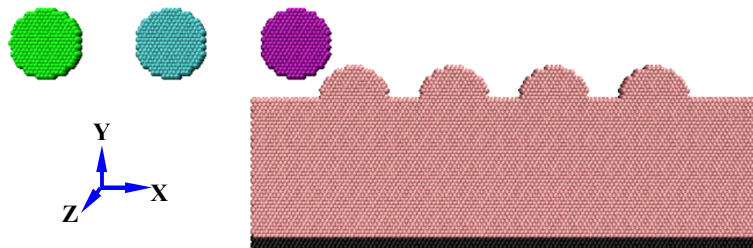


FIGURE 8.7
MD computation model

Three-body mechanical attrition employs a fine, loose abrasive to produce very fine surface texture and a high degree of flatness. Abrasive particles are projected with high velocity at the workpiece surface to remove surface films, such as oxides, and to impart to the surface a uniformly materials surface texture. Ultraprecision polishing has intense relationship with three-body attrition that accurately produces geometrical dimensional shapes in the nanometer order. Polishing based on three-body attrition is carried out without letting fine abrasive particles generate brittle fractures on the work surfaces, while removing these materials little by little only by means of plastic deformation, to finally produce a smooth mirror surface. For such polishing, fine abrasives of below 1 μm and pads of pitch, wax, synthetic resin, or artificial leather are used to realize smooth mirror finishing. Fine abrasive particles are retained on the pad surface resiliently and plastically, and the work surfaces are scratched microscopically. Polishing actions based on three-body attrition are smaller if compared with lapping, contributing to the successful applications to the brittle materials. The final surface integrity acquired using this technique is mainly depended on the microdynamic behavior of nanoparticles. The complex multibody interaction among nanoparticles and materials surface is different from interaction in the

macroscopic scale which makes the traditional classical materials machining theory can't accurately uncover the mystery of the surface generation process.

Molecular dynamics simulation, by virtue of its high temporal and spatial resolution, offers an ideal approach to gain insights into atomic scale process and understand their mechanisms. A remarkable enhancement in computational capability (computer hardware) and high performance computation techniques (parallel computation) has enabled us employing large scale classical MD method to investigate the nanometric attrition process. The atomic configuration of the system studied is illustrated in figure 8.7. Silicon atoms of particle and substrate are initially arranged in diamond cubic structure with a constant lattice parameter of 5.43 Å. The dimension of silicon workpiece is $180 \times 55 \times 50 \text{ \AA}^3$ along x, y and z directions. The moving speed is 100 m/s, the environment temperature is 293 K, the depth of cut is 8 Å, the particle diameter is 16 Å, the timestep is 2.5×10^{-15} s. For covalent systems, the Tersoff potential is used to depict the interaction between the silicon atoms and atoms of the abrasive particle as illuminated in the previous section.

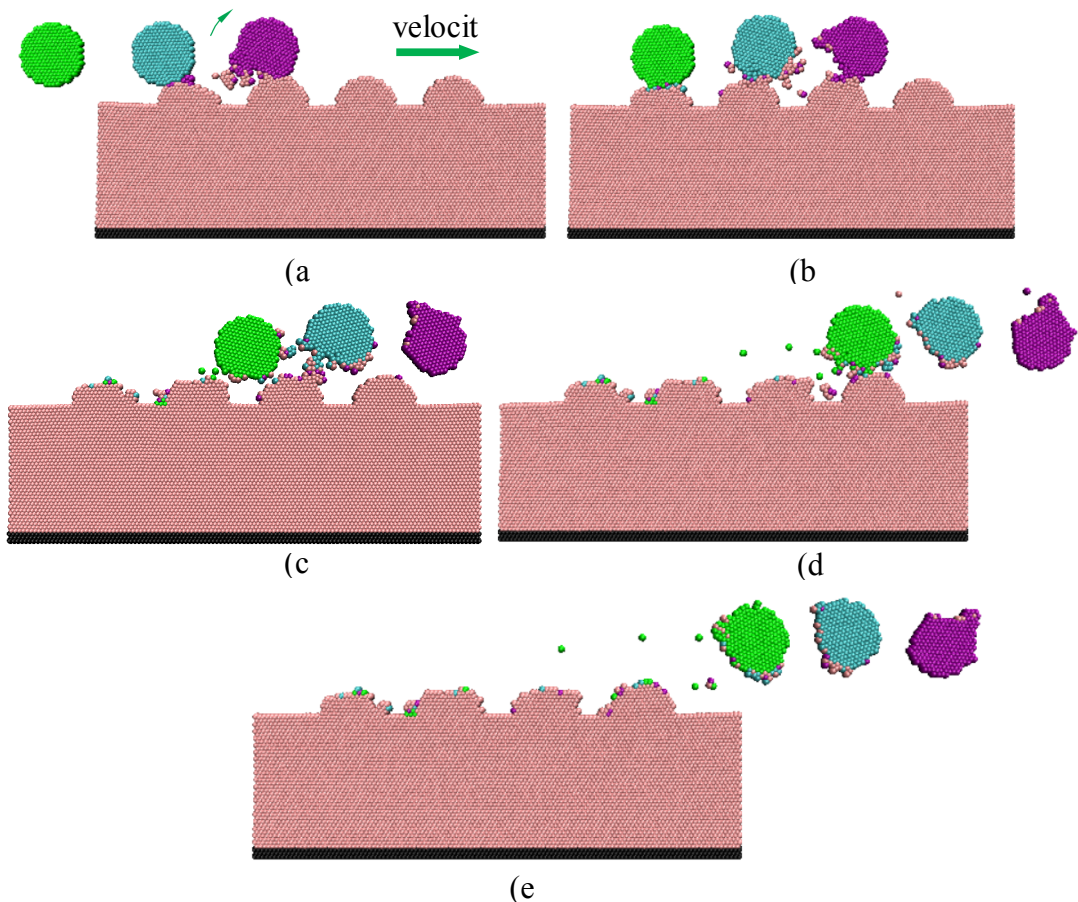


FIGURE 8.8

MD simulation of complex interaction among nanoparticles and substrate purple: particle1, cyan: particle2, green: particle3

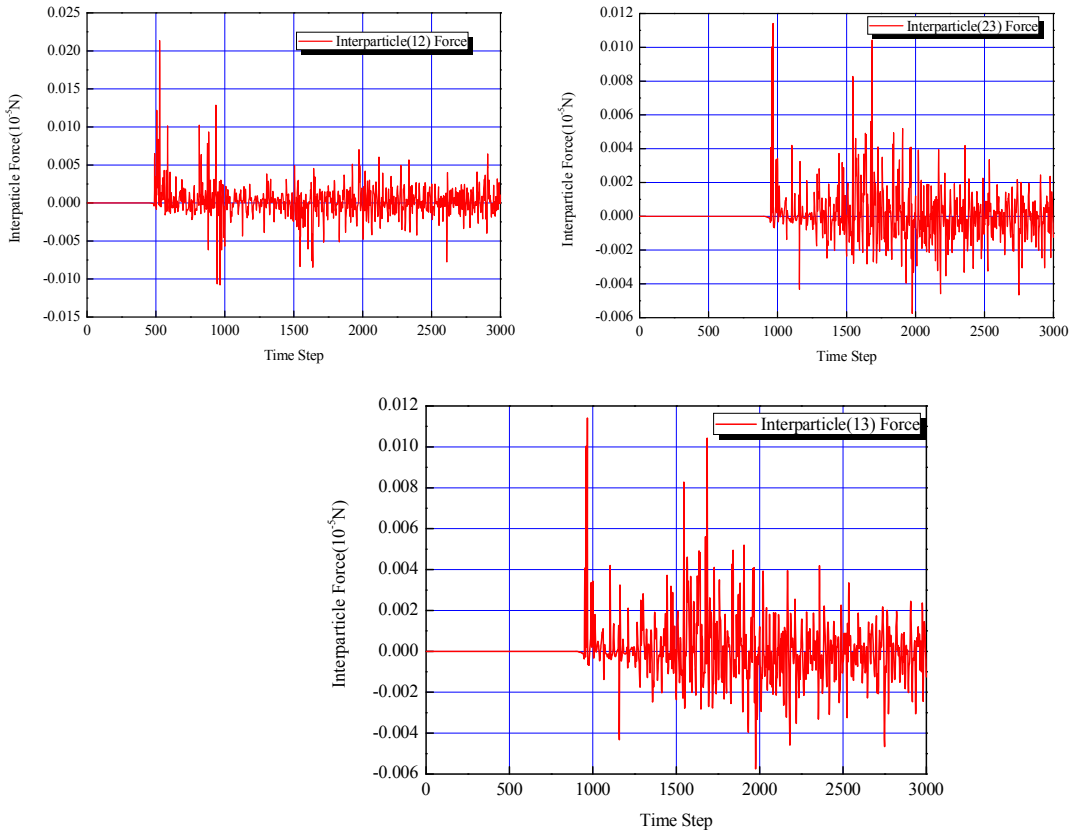


FIGURE 8.9
MD simulation of complex interaction among nanoparticles

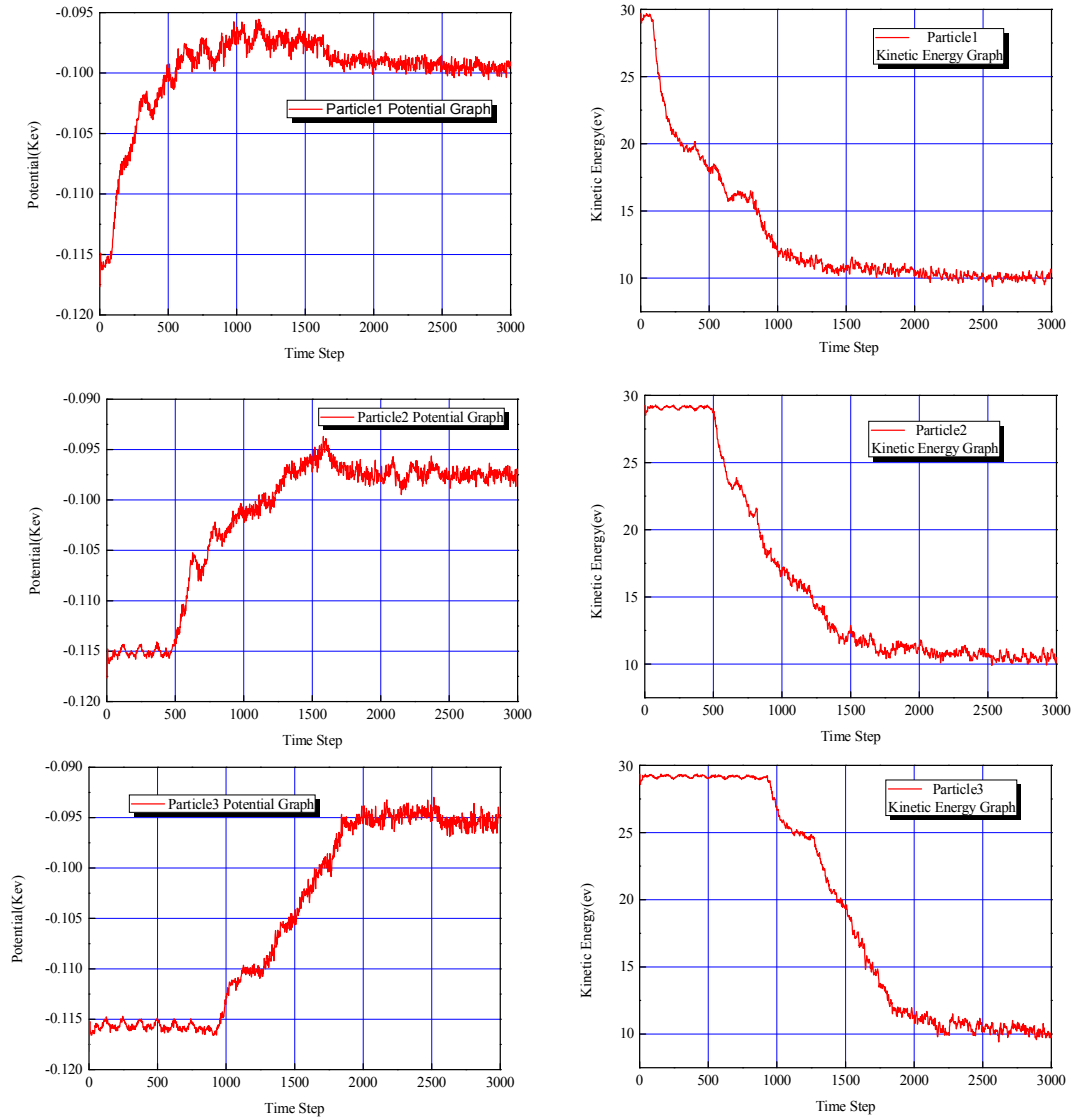


FIGURE 8.10
Variation of particle potential and kinetic energy

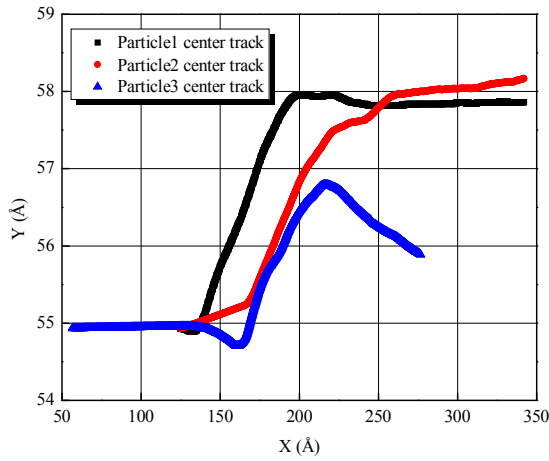


FIGURE 8.11
Particle center position

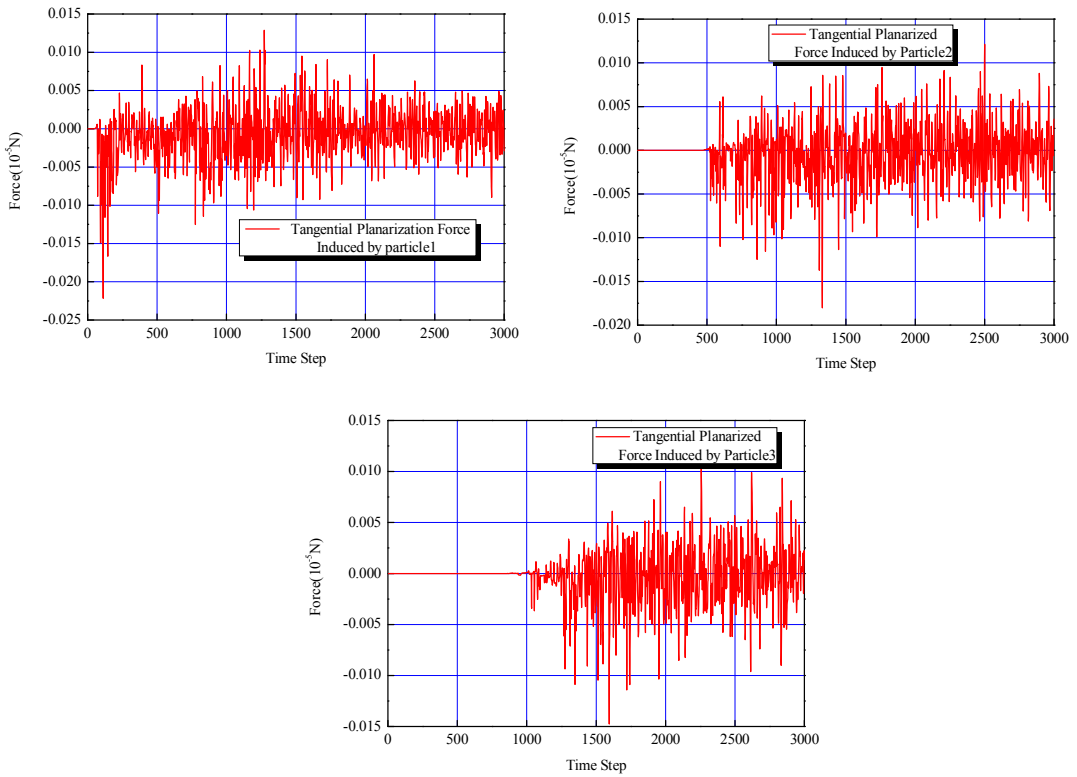


FIGURE 8.12
Tangential interacting force

The Velocity-Verlet method is a symplectic algorithm which can prevent the energy dissipation and have high computation efficiency and being adopted in this work.

Figure 8.13 gives the MD simulation of complex interaction among nanoparticles and single crystal silicon substrate. Firstly, these particles move parallel to the X direction but the rotational movement gradually been induced as the planarization process goes on. The translation plus rotation makes the nanoparticle behaved like micro-milling tool. But this tool is flexible and without definite shape. The tool should keep its dynamic behavior (micro & nanoscale inertia) between two discrete planarizing events if there is not external load exerted on it. As there is no rigid constraint which makes the tools gradually deviating from their original track, namely, the tool and substrate keep away from each other little by little.

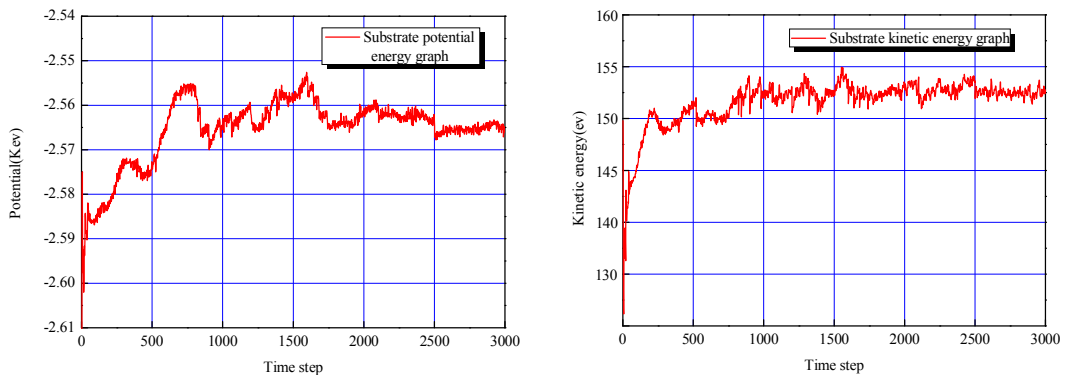


FIGURE 8.13
Substrate potential and kinetic energy graph

The particles were lifted after impacting the substrate materials. The animation movie also shows that only weak adhesion effect exists between substrate materials and particle2 (particle3). This dynamic trajectory leads to the first peak adjacent to the particles being planarized sufficiently while the last peak remains almost unplanarized. The interaction force between particle1 and particle2 increases after the two particles approach each other from 500 timestep (figure 8.9). Initially, the dynamic behavior of the two particles is influenced by the interaction between particle and the substrate which affect the surface planarization. This kind of substrate-particle interaction acts as integrate motion constraint because the substrate is fixed. It is just this relative kinematic motion realizing the surface planarization. The particle-particle interaction belongs to non-integrate motion constraint because the two particles also move independently. The interaction force between the two particles becomes stronger as they come closer and become a flexible constraint being exerted on the particles which makes the two particles moving like a unity. The same condition is also induced between particle2 and particle3 (figure 8.9). But the interaction force between this two particles increases after 1000 timestep which is different from the conditions between particle1 and particle2. The reason for this may be that after 500 timestep the particle1 begins to impact the substrate surface thus hindering it from moving ahead but the similar process takes 1000 timestep for particle2. Furthermore, the interaction force between particle1 and particle2 is much stronger than that of the force between particle2 and particle3 which means stronger force field generated between particle1 and prticle2. Finally, a new kind of flexible-many-body-tool (FMBT) is generated after 1000 timestep. The linkage between these particles belongs to internal flexible force field which is different from the macroscopic tools such as grinding wheel. This FMBT is not the same as the large atomic cluster because each body has its own geometry

and physical feature. The figure 8.11 also shows the center track of these particles after 1500 timestep which illuminates that they don't form larger cluster.

The polishing process can be considered as a process with energy release. A rough surface has high energy and a smooth surface has low energy. Figure 8.10 shows the variation of particle energy in the planarization process. The potential energy of particle1 gradually increased as it began to impact the substrate. The reason for this phenomenon is that the particle surface became rough and chemical active after the planarization. The kinetic energy of the particle1 is decreased because it doing work in the impacting process. Both the potential energy and the kinetic energy of the particles gradually come into a steady status at the end of impacting process. The graph of tangential interaction force (figure 8.12) illuminates the complex interaction between particle and substrate materials. Different from the beginning of impacting, there still interaction after the particle1 leaves the substrate. This phenomenon justifies that there are part of substrate materials adhere to the particle. This adsorptive materials may gradually evolves as outer surface layer of particle and act as the cutting tool to keep on planarized the substrate. The tangential interaction force gradually decreases and finally reaches a stable status which means there is little interaction between particle and substrate materials. The potential function gradually increased as the three-body process going on which means the deteriorating of surface roughness and the improving of surface planarization. This also means that the final planarized materials surface can only be achieved by synergic behavior of all particles using various means such as cutting, impacting, scratching, indentation and so on. The nanometer level global surface planarization can't be realized by single or small part of particles. The kinetic energy of substrate materials gradually increased as the attrition goes along as the external particles doing work to it.

X.4.2 MicroDynamic behavior of particles with different impact angle

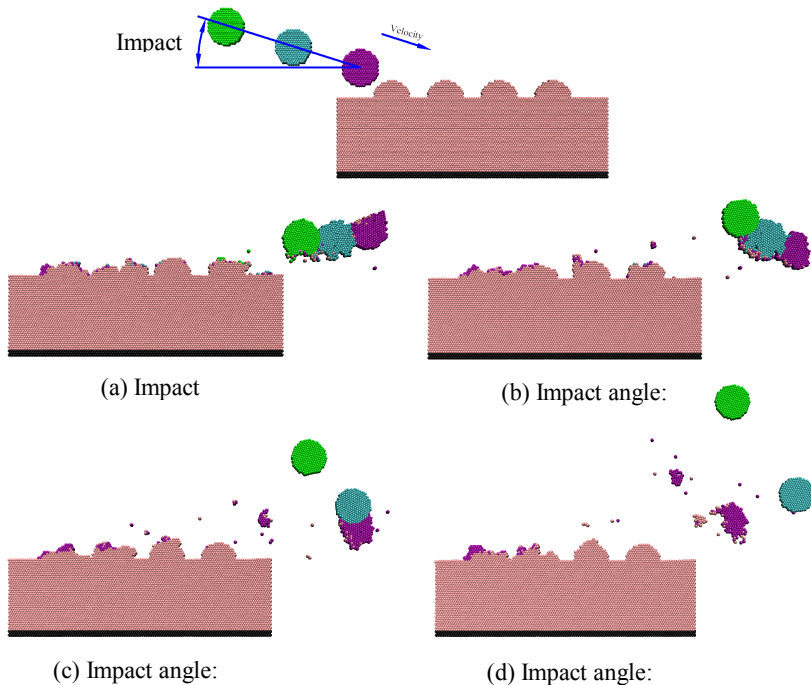
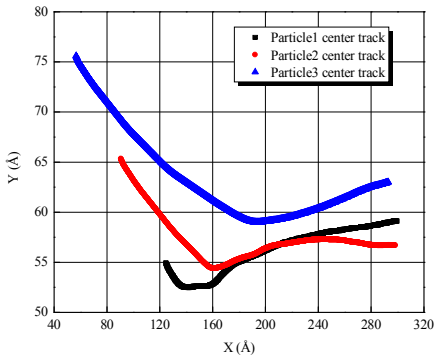
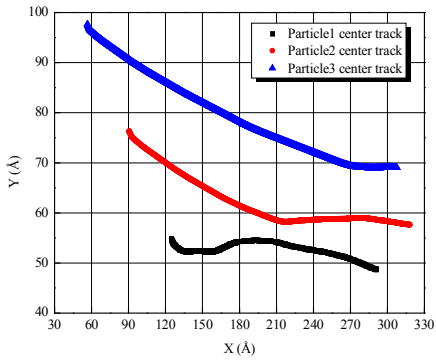
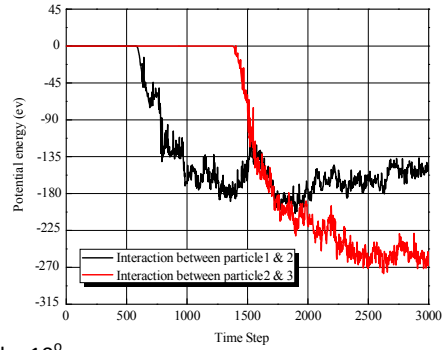


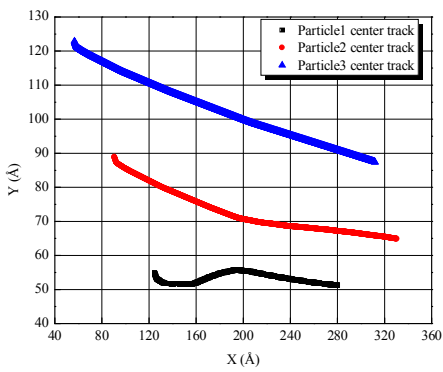
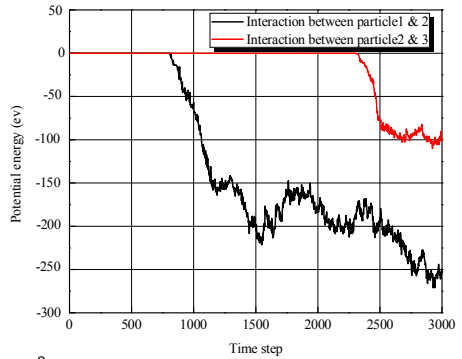
FIGURE 8.14 MD simulation of complex interaction among nanoparticles and substrate with different impact angle



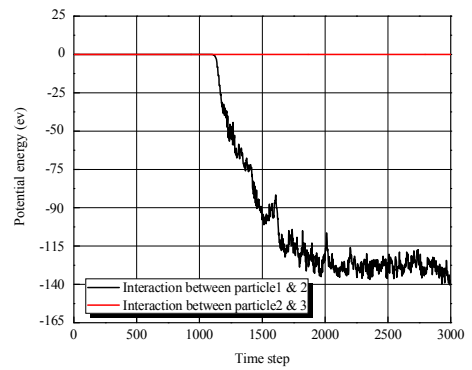
(a) Impact angle: 10°

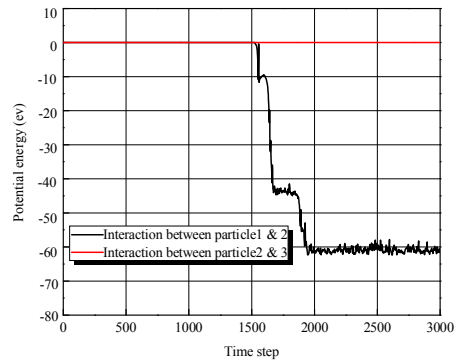
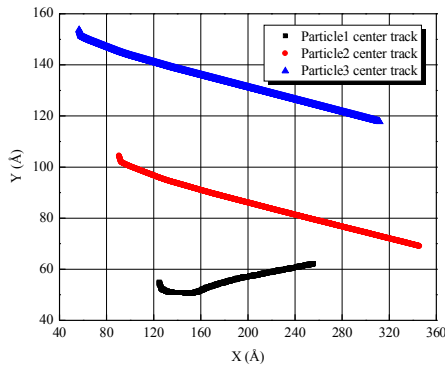


(b) Impact angle: 20°



(c) Impact angle: 30°





(h) Impact angle: 40°

FIGURE 8.15

Interaction nanoparticles and their center track with different impact angle

MD simulation results about the effects of different impact angle on nanoparticle dynamic behavior are shown in the figure 8.14-15. The particles begin to approach each other as the impact angle increasing from 5° to 15° . The larger atom cluster gradually comes into being while the impact angle in the range of $10^\circ \sim 15^\circ$. The particle center track shows that there exists inflection point where particle2 and particle3 experiences from gradually approaching to gradually separating. These particles ought to maintain their state of uniform motion unless being acted by an external force. The substrate materials may act as activate external load which change the status of particle dynamic behavior and the relationship among different particles. The particles with different impact angle generate different planarization surface. The particles with 5° impact angle induced the best planarization surface. Figure 8.14 shows that only the center track of the particle1 changed with different impact angle. That is to say, particle1 is the only effective tool of accomplishing the surface planarization process under the conditions of different impact angle.

The center track of all particles has inflection point in the three-body attrition process showed in the MD simulation. The particles ought to maintain their state of uniform motion unless external force acted upon it. The first inflection point should be the place where the planarization initialization. The surface force and other microscopic force may have a great influence upon the dynamic behavior of particles because this process happened in the microscopic scale. Complex tribology interaction (cutting, scratching, indentation, plough etc.) between particle and substrate as well as interaction among particle themselves is continually induced. The particles have to adjust its dynamic track accordingly. The center track of particle2 and particle3 gradually turned from irregular curve into straight line which illuminates the decreasing of their planarization behavior. The MD simulation in the figure 8.14 also provides intuitionistic description of this evolvement process. There are little wear or deformation of particle3 after the impact angle increased to 15° . This not means that no other external force acted on particle3 because its center track is not a straight line and there are still complex force field between particle2 and particle3 as shown in figure 8.15. The dynamic trajectory of particle3 gradually turned into straight line after the disappearing of external potential field, namely, after the impacted angle increased to 25° . The evolvement of center track of particle2 is similar with that of particle3. The center track of particle1 is different because it planarized the substrate materials under the conditions of different impact angle. There are stronger similarity about the dynamic trajectory of particle1 and particle2 with the 5° impact angle because stronger interaction potential field is buildup

between them. There are complex synergetic motion tendency between them. This tendency is gradually enhanced with the increasing of impact angles. These three particles are built into larger atomic cluster while the impact angle falls in the range of $10^{\circ}\sim 20^{\circ}$. Their dynamic trajectory exhibit amazing coherence. The cohesion strength among particles reaches the maximum value while the impact angle is 15° . After that the two body atomic cluster (particle1 and particle2) continually generated while the impact angle falls in the range of $25^{\circ}\sim 35^{\circ}$. There exists large similarity between their dynamic trajectories because of internal flexible constraint between them, namely, the effect of empirical force field. This flexible constraint gradually diminished after the impact angle increased to 40° . There are not any interaction exists among these particles after the impact angle increased to 45° and they finally interact with the substrate separately. Too large atomic clusters will induce surface damage and thus degrade the surface quality. The generation of larger atomic cluster may not entirely depend on chemical environment but have a tight relationship with the surrounding physical boundary conditions.

Conclusion

The research justifies that the influences of the mechanical actions of the abrasives (ultra-microcutting actions) that correspond to the cutting blade, and of the frictional actions of the pads can be considered as the factors that produce affected layers during mechanical attrition. The generation of fine plastic-cutting chips by the scratching behaviors of abrasives can be the influencing mechanism, which, however, given that the mechanical actions are extremely small, seems irrational unless other actions are taken into account. The mechanical attrition is a many body nanometer machining technology, and there exists complex interaction among particles as well as the interaction among particles and substrate materials. As this interaction falls into the nanometer regime, it is not downsizing but some new discipline and mechanism dominate the technology. Traditional continuum mechanics or experimental method can't give reasonable explanation about this microscopic dynamic process. It is seems that only combining all kinds of particle actions and various characteristic polishing conditions can the physical essence of mechanical attrition be discovered.

References

1. M. Petrica, C. Katsich, E. Badisch, F. Kreamsner, Study of abrasive wear phenomena in dry and slurry 3-body conditions, *Tribology International*, 2013, 64: 196~203
2. B. Stawarczyk, M. Ozcan, F. Schmutz, A. Trottmann, M. Roos, Two-body wear of monolithic, veneered and glazed zirconia and their corresponding enamel antagonists, *Acta Odontologica Scandinavica*, 2013, 71(1): 102-112
3. S. Kannan, H. A. Kishawy, M. Balazinski, Analysis of two- and three-body abrasive wear during machining of aluminium-based metal matrix composite, *International Journal of Materials & Product Technology*, 2013, 46(1): 81-94
4. S.A. Kumar, S.G.S. Raman, T.S.N.S. Narayanan, Influence of Surface Mechanical Attrition Treatment Duration on Fatigue Lives of Ti-6Al-4V, *Transactions of the India Institute of Metals*, 2013, 67(1): 137-141

5. J.F. Luo, D.A. Dornfeld, Effects of abrasive size distribution in chemical mechanical planarization: modeling and verification, *IEEE Transactions of Semiconductor Manufacturing*, 2003, 16(3): 469–476
6. F. Cemin, F.G. Echeverrigaray, A.C. Rovani, Influence of atomic and mechanical attrition on low temperature plasma nitriding of ferrous alloys, *Materials Science and Engineering: A*, 2010, 527(13-14): 3206-3209
7. A.L. Ortiz, J.W. Tian, L.L. Shaw, P.K. Liaw, Experimental study of the microstructure and stress state of shot peened and surface mechanical attrition treated nickel alloys, *Scripta Materialia*, 2010, 62(3): 129-132
8. J.M. Haile, *Molecular Dynamics Simulation-Element Method* (Wiley-Interscience, New York, 1997), 332-339