Materials Science and Engineering A 505 (2009) 65–69

Contents lists available at ScienceDirect

Materials Science and Engineering A

journal homepage: www.elsevier.com/locate/msea

# Molecular dynamics study of scratching velocity dependency in AFM-based nanometric scratching process

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ARTICLE INFO

*Article history:*
Received 24 July 2008
Received in revised form 27 October 2008
Accepted 28 October 2008

*Keywords:*
AFM
Scratching
Molecular dynamics
Scratching velocity

ABSTRACT

Three-dimensional molecular dynamics simulations are performed to investigate the AFM-based nanometric scratching process of monocrystalline copper. The effects of scratching velocities (1, 10, and 100 m/s) on the chip pattern, scratching resistance, dislocation movement, and workpiece deformation are studied. The results show that the scratching resistance increases with the increase in scratching velocity. The higher scratching velocity results in larger chip volume and closer chip shape with more amorphous structure. The dislocations move well-regulated for lower velocities (1 and 10 m/s) than that for larger one (100 m/s). The area of workpiece material deformation region beneath the tool edge decreases with the increase in scratching velocity.



## 1. Introduction

With advancements of scanning probe microscopy (SPM) techniques, the atomic force microscope (AFM)-based nanometric scratching method is proposed to fabricate micro/nano-components/devices in micro-electro-mechanical system (MEMS) and nano-electro-mechanical system (NEMS) [1,2]. The machining scale for this method is determined solely by the geometry of AFM probe, thus the resolution of this technique can reach at least the same scale as the AFM probe, material removal of few nanometers can be achieved. Materials' physical properties change with a reduction in its size in the field of nano-scale science, and the established conventional cutting mechanism cannot be applied to analyze the AFM-based nanometric scratching process on the atomic scale. Hence, experimental studies and theoretical analysis of material removal mechanism in AFM-based nanometric scratching process, such as friction and wear, scratching force, elastic and plastic deformation, etc., are required to facilitate the development of high precision machining micro/nano-components/devices. Due to many modern developments in the field of computer modeling technology, experimental studies of material removal mechanism on the atomic scale are now supplemented with numerical simulation studies, which allow us to explore detailed deformation process and properties of materials together with the scientific visualization technique. The most widely used method is the molecular dynamics (MD) simulation, which has been confirmed to best be the suit for analyzing nanometric machining process.

The MD simulation method was first adopted to investigate the nanometric cutting of copper with a diamond tool by a research group at the Lawrence Livermore National Laboratory (LLNL) in the late 1980s [3]. This work leads other researchers to explore and extend MD simulation to many other machining applications. Komanduri et al. conducted MD simulation of nanometric cutting under different cutting conditions to investigate burr formation and exit failure in metals [4]. Tanaka et al. conducted MD simulation to analyze the nanometric deformation behavior in three-point bending of defect-free monocrystalline silicon [5]. Fang et al. proposed a new model based on extrusion to understand how materials are removed from workpiece in nano-cutting, which was different from the shearing mechanism in conventional cutting [6].

However, an issue that can be drawn from reviewing the literatures of MD simulation of nanometric machining processes is that, in order to accomplish MD simulation of nanometric machining processes within an acceptable computational time, generally high machining velocities were utilized in previous works, such as 500, 200, 100 m/s, etc. Due to limited computational power, these works were not exactly over the same length scale and time scale with experimental studies, in which machining velocities were much lower being of the order of $\mu m/s$. The higher machining speed would result in the miss of some diffusive transitions of atoms during the machining process [7]. Therefore, in order to obtain more detailed information about nanometric machining process,

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doi:10.1016/j.msea.2008.10.049

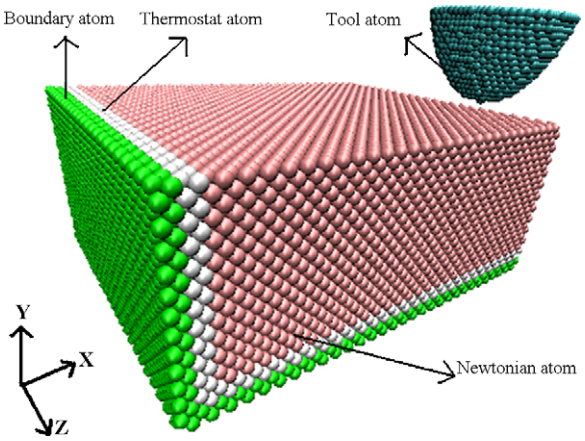


**Fig. 1.** MD simulation model of AFM-based nanometric scratching.

it is necessary to conduct MD simulation with lower machining velocity. Furthermore, it is an important issue to investigate the effect of machining velocities on the MD simulation of nanometric scratching process.

Therefore, in this paper, three-dimensional MD simulations of the AFM-based nanometric scratching process are conducted, an ultra low scratching velocity of 1 m/s is simulated. Simultaneously, two larger scratching velocities (10 and 100 m/s) are also simulated to investigate the effects of scratching velocity on AFM-based nanometric scratching process. Chip pattern, scratching resistance, dislocation movement, and workpiece deformation are studied.

## 2. Simulation methodology

As shown in Fig. 1, the AFM-based nanometric scratching consists of a monocrystalline copper workpiece and an AFM diamond pin tool. The scratching is simulated along the [−1 0 0] direction of the (0 1 0) surface of workpiece.

The copper workpiece has a dimension of $30a \times 12a \times 24a$ (a is the lattice constant of copper, 0.361 nm) and contains 36,600 atoms. Workpiece consists of three types of atoms such as boundary atoms, thermostat atoms, and Newtonian atoms. Boundary atoms are frozen on their perfect lattice sites to reduce the edge effects. Both of the thermostat atoms and Newtonian atoms' motion obey the Newton's second law, and are determined by the direct integration of the classical Hamiltonian equations of motion using Velocity-Verlet method. System's initial temperature is 293 K. As considerable energy is added to thermostat atoms during cutting process, heat dissipation is carried out during the MD simulation process to keep thermostat atoms at constant temperature of 293 K, whose velocities are adjusted at every five computational time steps using the velocity rescaling method. Periodic boundary condition is maintained along *Z*-direction to reduce effects of simulation scale.

The AFM diamond pin tool utilized in current study has a configuration of ellipse shape. It is constructed with perfect diamond atomic lattices, consisting of 1943 atoms with a radius of 2.3 nm. In view of the significant higher hardness of diamond than copper, the AFM pin tool is treated as a rigid body in current MD simulations.

For the Cu–Cu atomic interactions between workpiece atoms, the well established embedded atom method (EAM) potential for copper constructed by Foiles is utilized, which can give a realistic description of the behavior and properties of metal [8–10]. It has been used successfully in previous study [11]. For EAM potential, the total atomic potential energy of a system is expressed as Eq. (1):

$$E_{tot} = \frac{1}{2}\sum_{ij}\phi_{ij}(r_{ij}) + \sum_{i}F(\rho_i)_i \tag{1}$$

where $\phi_{ij}$ is the pair-interaction energy between atoms *i* and *j*, and $F_i$ is the embedded energy of atom *i*. $\rho_i$ is the host electron density at site *i* induced by all other atoms in the system, which is given by Eq. (2):

$$\rho_i = \sum_{j\neq i}\rho_j(r_{ij}) \tag{2}$$

For the Cu–C interaction between workpiece atoms and tool atoms, the Morse potential is used, which is relatively simple and computationally inexpensive compared to the EAM potential. The Morse potential is written as Eq. (3):

$$E_{tot} = \sum_{ij}D_0[e^{-2\alpha(r-r0)} - 2e^{-\alpha(r-r0)}] \tag{3}$$

where $E_{tot}$ is a pair potential energy function; $D_0$ is the cohesion energy; $\alpha$ is the elastic modulus; *r* and $r_0$ are the instantaneous and equilibrium distance between atoms *i* and *j*, respectively. The cutoff radius of the Morse potential is chosen as 0.9025 nm, which ensures that the calculations will not consume large amounts of computational time. In the current study, the Morse potential parameters are adopted as $D_0 = 0.087$ ev, $\alpha = 51.4\ \text{nm}^{-1}$ and $r_0 = 0.205$ nm.

The force acting on an individual atom *i* resulting from the interaction of all other atoms can be derived from above potentials:

$$F_i = -\sum_{j=1}^{N}\nabla_i E(r_{ij}) = m_i\frac{\mathrm{d}^2 r_i(t)}{\mathrm{d}t^2} \tag{4}$$

where $F_i$ is the resultant force on atom *i*, $m_i$ is the mass of atom *i*, $r_{ij}$ is the distance between atoms *i* and *j*, and *N* is the total number of atoms. In current study, two force components, as scratching force and normal force are studied. The scratching force is defined as the force paralleling to the scratching direction, the normal force is defined as the force paralleling to the *Y*-direction.

In the current study, the centro-symmetry parameter (CSP) is adopted to identify dislocation movements. The CSP is a useful measure of the local lattice disorder around an atom, and can be used to characterize whether the atom is part of a perfect lattice, a local dislocation, or at a surface. The value of the CSP will be 0.0 for atoms in a perfect face centered cubic (FCC) lattice. The CSP is computed using the following formula constructed by Kelchner et al.:

$$P = \sum_{i=1}^{6}|\vec{R}_i + \vec{R}_{i+6}|^2 \tag{5}$$

Where $\vec{R}_i$ and $\vec{R}_{i+6}$ are the vectors from the central atom to the opposite pair of nearest neighbors [12]. The workpiece atoms are colored according to the CSP values by the Atomeye code [13].

**Table 1**
Computational parameters of MD simulations.

| Configuration | Workpiece: copper (FCC) | Tool: diamond (rigid) |
|---|---|---|
| Dimensions | $30a \times 12a \times 24a$ (a, lattice constant, 0.361 nm) | Radius: 2.3 nm |
| Number of atoms | 36,600 | 1943 |
| Time step | 1 fs | |
| Initial temperature | 293 K | |
| Uncut chip thickness | 1 nm | |
| Cutting length | 8 nm | |
| Cutting speed | 1, 10, and 100 m/s | |
| Cutting directions | [1 0 0] on (0 1 0) surface | |