A Three-Dimensional Molecular Dynamics Modeling of Nano-Cutting Processes

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Abstract

This paper proposes a three-dimensional atomistic model to analyse the nano-cutting process of a monocrystal copper by a diamond tool. With the aid of the molecular dynamics analysis, the Morse potential was used to calculate the interatomic forces between any pair of atoms. The dislocation interactions and residual defects during and after nano-cutting were studied. Compared with the existing two-dimensional models that are unable to describe dislocation interactions and residual defects, the present model offers a new insight into the nano-cutting processes and provides much more reliable results.

Key Words: Nano-cutting, Molecular dynamics, Dislocations, Residual defects, Three-dimensional modeling

1. Introduction

Nano-cutting is one of the key techniques for manufacturing ultra-precision components. Hence, the full understanding of the mechanisms of nano-cutting is of primary importance to the further development of nanotechnology and precision engineering. Based on the molecular dynamics analysis, a number of nano-cutting models via computer simulation have been developed and served as a useful tool to understand the deformation process of workpieces. However, previous studies are mainly two-dimensional [1-6] such that the exact mechanisms of initiation and evolution of dislocations and exchanges of Burger's vectors during cutting cannot be investigated properly. In a two-dimensional model, in fact, a single and isolated dislocation can move to the workpiece surface with a very low resistance, because dislocation lines in the model are always in parallel with each other and interactions of dislocations do not occur. This differs significantly from what happens in a real cutting process.

The present paper proposes a three-dimensional atomistic model to investigate the nano-cutting process of a system composed of a diamond tool and a copper workpiece. Using the molecular dynamics analysis, a three-dimensional Morse type function of interatomic potential is used to generate the interatomic forces between any pair of atoms. Particular attention is paid on the exploration of dislocation interactions during cutting and on the development of residual surface and sub-surface defects.

2. Three-Dimensional Modeling

Molecular dynamics (MD) analysis is a microscopic method to analyse the behaviour of solids from an atomistic point of view. Using this method, progressive motion including lattice vibration of individual atoms in the solid model can be traced by sequentially solving the differential equations of motion of the atoms.

To simulate a nano-cutting process adequately, let us use a three-dimensional Morse interatomic potential to generate the interatomic forces between any pair of workpiece atoms and workpiece-tool atoms in the model. For simplicity, we first assume that the diamond cutting tool is rigid. The Morse potential between two atoms, $E(r)$, can be written as

$$E(r)=D[\exp\{-2a(r-r_0)\}-2\exp\{-a(r-r_0)\}] \quad (1)$$

where D, a and r_0 are materials constants and can be determined by the cohesive energy, the elastic modulus, C_{11}, and the equilibrium interatomic distance. For the copper-diamond junction, while the elastic modules and equilibrium interatomic distance is assumed to be the average value of those of copper and diamond, the cohesive energy is estimated from an experimental value for separation energy of the junction in an ultra-high vacuum. The parameters used in the computer simulation are listed in Table 1 [1-2].

Table 1. Parameters in the Morse potential function

	Copper-Copper	Copper-Diamond
a (nm^{-1})	13.59	51.40
D (eV)	0.342	0.087
r_0 (nm)	0.287	0.205

For a simulation with a long cutting distance, the moving control volume method is necessary when

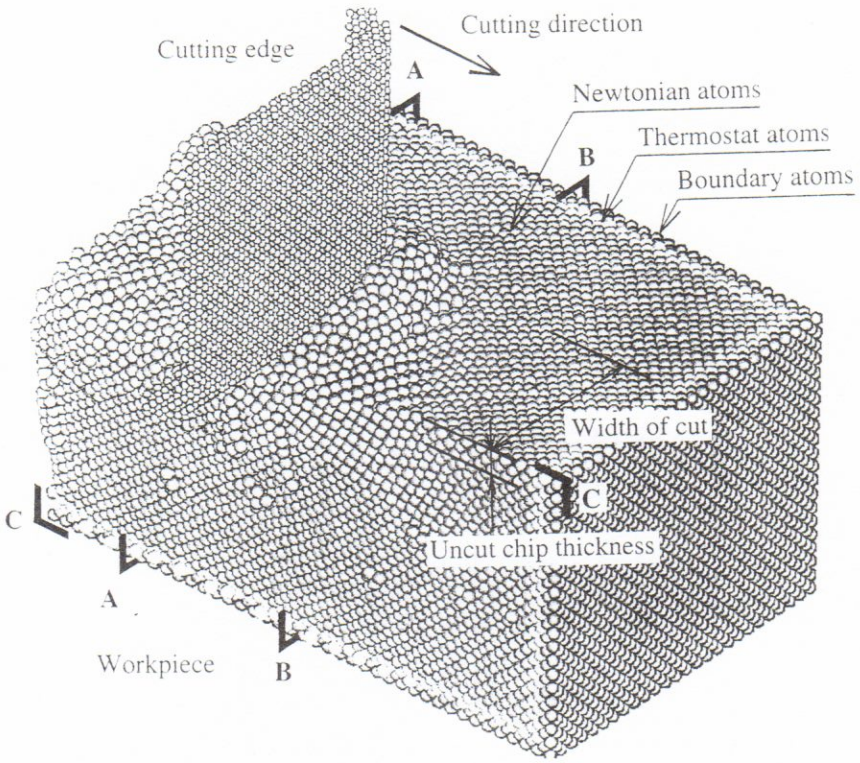


Fig. 1 A schematic model of nano-cutting using molecular dynamics simulation

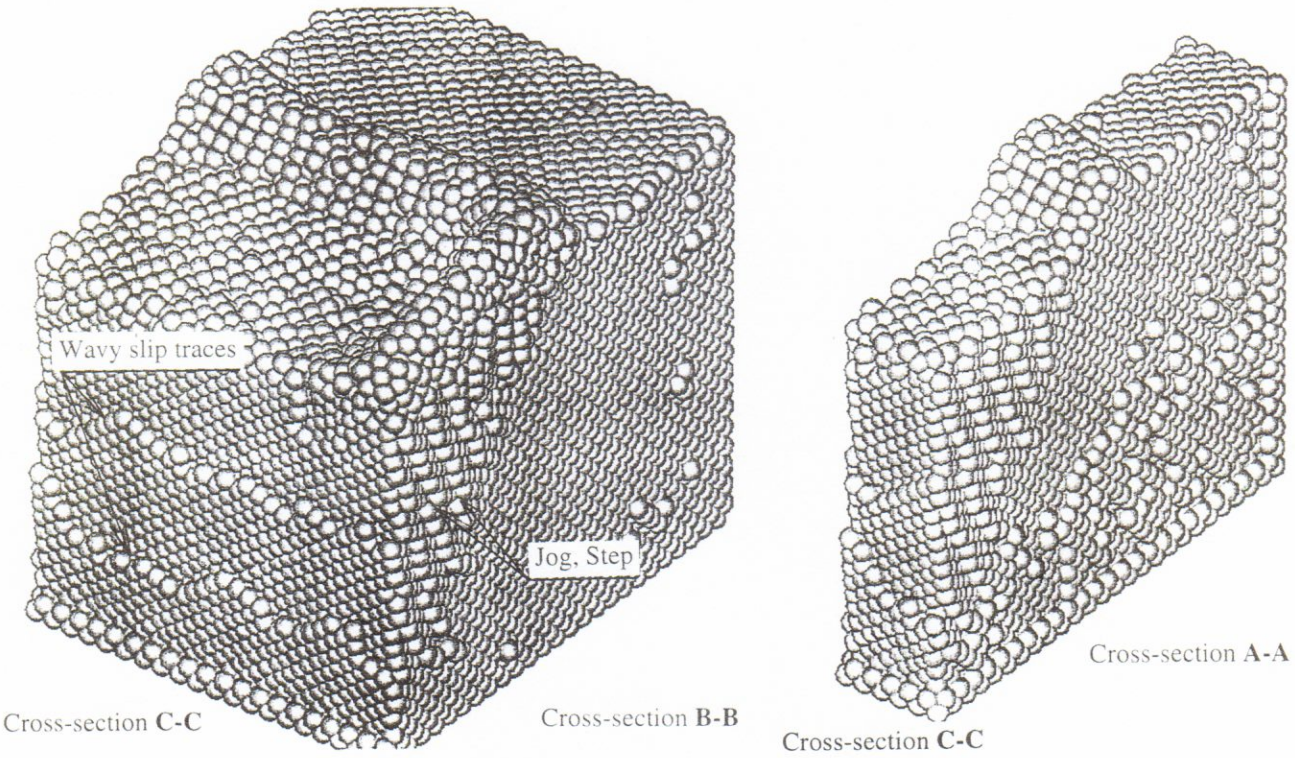
using a relatively small model, in which the workpiece atoms behind the cutting zone with a negligible effect on the motion of the atoms are removed from the model and new atoms are added simultaneously ahead of the cutting zone. In this way, the atomic model always keeps a constant volume and the cutting zone is mostly located at the center of the model. Hence, the boundary effect can be adequately eliminated even with a relatively small control volume.

Moreover, a calibration of thermal conductivity, when using the MD for a nano-cutting analysis, is essential because of the following reasons. The MD method can effectively simulate the propagation of force or deformation, because the displacement of an atom directly changes the interatomic potential between the atom and its neighbouring ones and causes an energy transfer. As the transfer is carried out from potential energy to kinetic energy in an MD simulation, the generation of heat in terms of the increase in lattice vibration energy due to dislocation movement can be well simulated. However, unlike the case in covalent solids, where heat is transmitted by means of lattice vibration, the thermal conductivity in metals is mainly governed by the mobility of electron. Thus metals usually show much higher thermal conductivity than that estimated by an MD simulation. Therefore, to study properly the thermal field in nano-cutting metals, the gradient in thermal field should be "scaled" or "adjusted" to make the MD simulation consistent with that obtained by the continuum theory of thermal conductivity[4].

Table 2. Parameters in computer simulation

Workpiece	Monocrystal copper (Assuming that the three-dimensionalMorse potential applies)
Tool	Rigid diamond
Configuration	Orthogonal cutting (see Fig. 1)
Cutting speed, v	200 (m/s)
Uncut chip thickness, d	0.5 (nm) (see Fig. 1)
Cutting width, w	4 (nm) (see Fig. 1)
Edge radius of the cutting tool, R	0.08 and 1 (nm)
Rake angle, α	0 (degree)
Total cutting distance simulated, l	100 (nm)
Initial bulk temperature of the workpiece	293 (K)
Time step for integrating the equations of motion	10 (fs)

To accommodate the problems discussed above, we construct our three-dimensional model in such a way that the Newtonian atoms are surrounded by two layers of thermostat atoms which are further bounded by two layers of boundary atoms, as shown in Fig. 1. The static boundary atoms are fixed and rigid. The motions of all of the Newtonian atoms during a cutting process can



(a) Cross-sections under the cutting edge

(b) Residual defects

Fig. 2 Cross-sections of the workpiece
(v=200 m/s, R=1 nm, d=0.5 nm, w=4 nm, l=100 nm)

then be numerically monitored by solving the equations of motion instantly using the Verlet's algorithm [7]. The total kinetic energy of the thermostat atoms is always kept a constant, which means that the heat generated by cutting escapes from the model through the thermostat atoms.

The initial velocity of each atom is statistically given by the Maxwell-Boltzman's distribution corresponding to the initial bulk temperature of the workpiece. Table 2 summarises the parameters used in our cutting simulation.

3. Results and Discussion

3.1 Dislocation interactions and residual defects

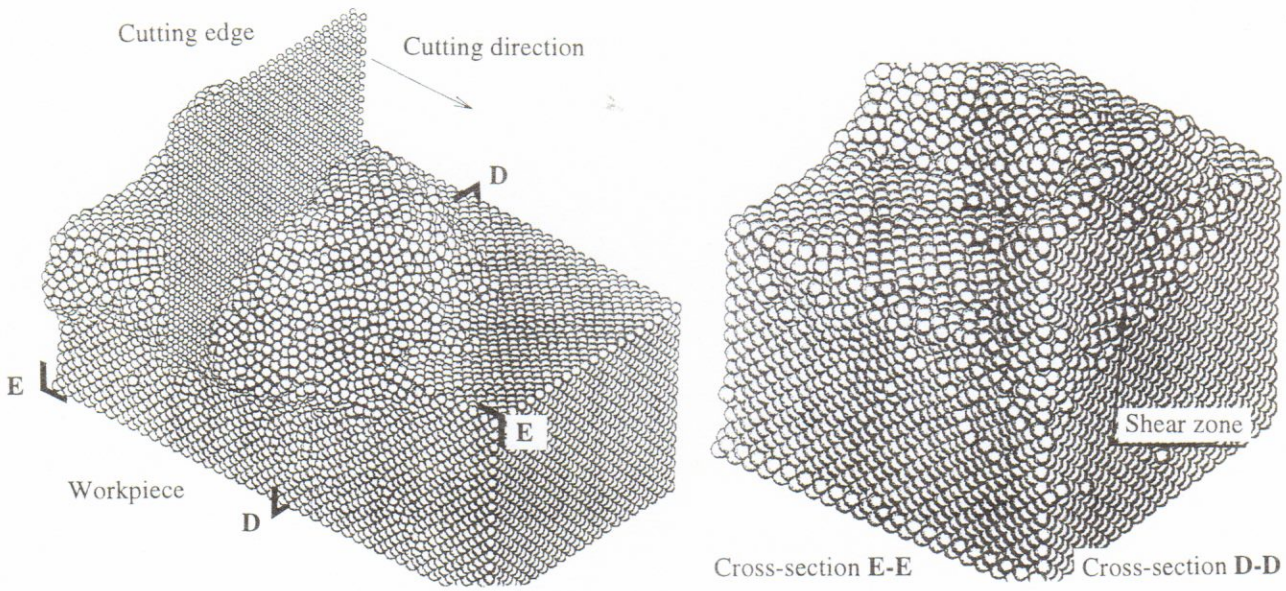
Figure 2 shows the cross-sections of the workpiece and the deformed layer after a cutting at d=0.5 nm with R=1 nm. Complicated elastic and plastic deformation in the workpiece appears due to the mechanical action of the cutting edge. Some dislocations generated on the tool-workpiece interface grow and penetrate into the subsurface of the workpiece. After the cutting edge moves away from the deformed zone, elastic recovery takes place, the dislocations in the subsurface experience an unloading movement, and finally many of them are arrested in the surface and subsurface.

Wavy slip traces caused by cross-slip are observed on the cross-sections parallel to the cutting direction (e.g. cross-section **C-C** in Fig. 2a). This indicates that the moving screw dislocations change their slip planes. It is clear that screw dislocations can be simulated using the molecular dynamics analysis with the three-dimensional Morse type function of interatomic potential.

Jogs or steps on the same slip plane are observed on the cross-sections perpendicular to the cutting direction. The jogs are generated by the interactions of the non-parallel dislocations, see for example cross-section **B-B** in Fig. 2a.

3.2 Effect of cutting edge sharpness on the residual defects

To understand the effect of the cutting edge sharpness on the residual defects, the cutting simulation is made for another cutting edge sharpness (R=0.08 nm). Figure 3 shows the effect of cutting edge sharpness on the residual defects with the cutting edge radius of an atomic diameter of diamond. As R increases, the size of deformed volume in the shear zone and the density of residual defects after cutting increase. These indicate that the cutting edge sharpness is one of the important factors



(a) Chip formation when cutting the monocrystal copper

(b) Cross-sections under the cutting edge

Fig. 3 Effect of cutting edge sharpness on the residual defects
(v=200 m/s, R=0.08 nm, d=0.5 nm, w=4 nm, l=100 nm)

Table 3 Comparison of two-dimensional and three-dimensional cutting simulation with Morse potential using MD

	Two-dimensional simulation	Three-dimensional simulation
Modeling	Assumed (111) plane model	Three-dimensional model of any crystal direction
Dislocation	Assumed edge dislocation Parallel dislocation	Edge, screw, mixed dislocation Parallel and Non-parallel dislocation
Dislocation motion without reactions	Straight	Straight Cross-slip, (Dislocation climb)
Dislocation interaction	Impossible	Jog, Step
Dislocation reactions	Exchange of Burger's vector	Formation of a third dislocation from dislocation reactions Partial dislocations
Other defects	Vacancy Grain boundary (Tilt boundary)	Vacancy Grain boundary (Tilt boundary) (Twin) (Stacking fault)
Deformed layer	Perfect crystal	Residual defects

in terms of residual defects, and that the sharper the cutting edge the smaller the deformation layer.

3.3 Comparison with the existing two-dimensional analyses

There are some disadvantages when using two-dimensional analyses. For instance, it is impossible to simulate screw and mixed dislocations, non-parallel dislocations, dislocation interactions and residual defects. Table 3 shows the comparison of two-dimensional and three-dimensional cutting simulation with Morse potential for interatomic potential by MD.

Figure 4 shows the deformed region around a cutting edge in plane (111) of a monocrystalline copper workpiece with the two-dimensional analysis. The displacement of atoms from the initial position is shown in enhanced manner by enlarged circles for easier understanding [5,6]. Comparing Fig. 2 with Fig. 4, it found that the process of generation and development of dislocations in the workpiece is more complex than those predicted by the two-dimensional model. The depth of deformation zone presented by the two-dimensional model is smaller. This is probably caused by the implicit restrain in two-dimensional models, where the motions of

atoms are limited in a plane such that the resistance to dislocation motion has been highly increased.

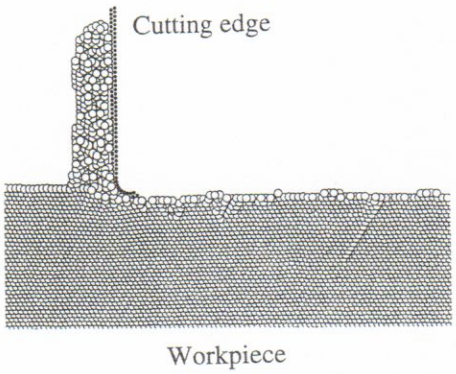


Fig. 4 Deformation prediction with a two-dimensional model when cutting the monocrystal copper (v=200 m/s, R=1 nm, d=0.5 nm, l=30 nm)

4. Conclusions

Compared with the previous two-dimensional modeling, the present three-dimensional cutting analysis shows the following distinct advantages:

(1) The residual defects on the surface and in the sub-surface of a workpiece can be revealed with the Morse potential.

(2) Cross-slip of moving screw dislocations and jogs and steps caused by dislocation interactions can also be explored easily.

(3) The three-dimensional model also indicates that a two-dimensional model would usually underestimate the size of the deformation zone subjected to nano-cutting.

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