Molecular Dynamics Simulations of Atomic Scale Indentation and Cutting Process with Atomic Force Microscope*

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This paper describes the effect of the material used for a tool on atomic scale indentation and cutting mechanisms of metal workpieces, by means of molecular dynamics simulations. The interatomic force between the tool and workpiece is assumed to be a two-body interatomic potential using parameters based on the *ab-initio* molecular orbital calculation for a (Cr, Ni)-(C, Si)₆H₉ atom cluster. Molecular dynamics simulated the atomic scale indentation and cutting process of the chromium and nickel workpieces using the diamond, silicon and diamond-like carbon (DLC) tools. The diamond and DLC tools formed the indentation mark. Young's modulus of the chromium and nickel in indentation simulations was larger than that in experiments. This was qualitatively explained by the effect of the surface energy for the workpiece on the elastic modulus. The machinability of the chromium and nickel with the diamond tool was better than that of the silicon tool in atomic scale cutting simulations. The depth of the cut for the workpieces in nano scale cutting experiments with AFM, was similar to that in atomic scale cutting by molecular dynamics simulations.

Key Words: Molecular Dynamics, *ab-initio* Molecular Orbital Calculation, Atomic Force Microscope, Indentation, Cutting, Young's Modulus, Machinability

1. Introduction

Atomic force microscope (AFM) is an advantageous microscope for measuring the surface roughness and frictional property of various materials on a nano or atomic scale. AFM has also been used for a nano indentation and cutting test due to its high accuracy positioning control system on an atomic scale⁽¹⁾⁻⁽³⁾. Understanding mechanisms of a nano indentation and cutting process with AFM is essential for the improvement of the test procedure and test accuracy. However, the indentation and cutting mechanisms on a nano or atomic scale have not been well understood since clarifying the mechanisms in experiments is so difficult.

Molecular dynamics (MD) simulation is useful for

understanding the atomic scale deformation mechanism of a workpiece during the indentation and cutting process. Especially, three-dimensional (3D) MD analyses can reveal the effect of crystal orientation on the indentation and cutting mechanism⁽⁴⁾. The surface roughness of a workpiece can also be measured by a 3D MD analysis. In this study, we carried out 3D MD simulations of the indentation and cutting using deformable tool models. So far, some MD analysis of an atomic scale indentation and cutting was performed using a rigid tool model⁽⁵⁾⁻⁽⁷⁾. These analyses have overestimated the deformation of a workpiece during the indentation or cutting since the analyses did not take account of the tool deformation. Three-dimensional MD analyses using a deformable tool must be carried out to understand deformation mechanisms of a workpiece during the atomic scale indentation or cutting process with high accuracy.

The objective of this paper is to study the indentation and cutting mechanisms on an atomic scale by means of 3D MD simulation. This study focuses on the effect of material used for a tool on the

* Received 22th December, 1998. Japanese original: Trans. Jpn. Soc. Mech. Eng., Vol. 64, No. 625, A (1998), p. 2263-2270 (Received 13th October, 1997)

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Fig. 1 Molecular dynamics simulation models

deformation mechanism of a metal workpiece during atomic scale indentation and cutting. Three-dimensional MD simulations of the indentation and direct cutting were carried out under the canonical (N, V, T ; N : number of atoms, V : volume, T : temperature) ensemble⁽⁸⁾, corresponding to constant-temperature experiments, for chromium and nickel single crystals using three kinds of deformable pin tools. Young's modulus of the workpieces was evaluated by using load-penetration depth curves obtained in indentation

Table 1 Molecular dynamics simulation condition

Workpiece	Chromium	
	Mass of Cr atom	$10.644 \times 10^{-26} \text{ kg}$
	Number of Cr atoms (for indentation analysis) (for cutting analysis) The top surface	4416 9216 (110)
	Nickel	
	Mass of Ni atom	$9.834 \times 10^{-26} \text{ kg}$
	Number of Ni atoms (for indentation analysis) (for cutting analysis) The top surface	5184 10496 (111)
Pin tool	Tip radius	5nm
	Diamond	
	Mass of C atom	$2.012 \times 10^{-26} \text{ kg}$
	Number of C atoms	2395
	Silicon	
	Mass of Si atom	$4.704 \times 10^{-26} \text{ kg}$
	Number of Si atoms	673
	DLC coating on Si tip	
	Number of C atoms	1037
	Number of Si atoms	356
	Density	3.0 g/cm^3
Indentation condition	Temperature	300K
	Time step	0.5fs
	Indentation speed	200m/s
	Moving distance of pin tool	8.3 Å
Cutting condition	Normal load of diamond of silicon	300nN 200nN
	Temperature	300K
	Time step	0.5fs
	Cutting speed	200m/s

simulations. The cutting force acting on a tool during the direct cutting simulations were examined for the machinability of the workpieces. Nano scale cutting experiments with AFM were also carried out to study the machinability of the workpieces. Analytical results were compared with the nano-scale cutting experiments.

2. Analytical Procedure

2.1 Molecular dynamics simulation

Three-dimensional MD indentation and cutting simulations were carried out for the chromium and nickel single crystals using the diamond, silicon and diamond-like carbon (DLC) pin tools. The DLC tool was modeled by depositing carbon atoms arbitrarily on a silicon substrate. The top surface of workpieces used here was the chromium (110) and nickel (111) surface. Atoms on the bottom surface of the workpieces were fixed in the x -, y - and z -directions (Fig. 1). The indentation simulations were conducted under the tool displacement controlled condition with the indentation speed at 200 m/s. The pin tools in the indentation were moved from their initial position to the distance of -0.83 nm in the z -direction. The cutting process was simulated under the normal load of pin tools controlled condition with the load at 200 nN and 300 nN. The other MD simulation parameters are listed in Table 1.

The interatomic potential of chromium (Cr) atoms

and that of nickel (Ni) atoms were assumed to be the Finnis-Sinclair (FS) potential⁽⁹⁾ and the Embedded Atom Method (EAM) potential⁽¹⁰⁾, respectively. The interatomic potential of carbon (C) and silicon (Si) atoms for the diamond, silicon and DLC tools was assumed to be the three-body potential proposed by Tersoff⁽¹¹⁾. A many-body potential as the FS, EAM and Tersoff is useful potential to solve problems of surface energies, surface geometry, grain boundaries, internal voids and fracture process in several materials⁽¹²⁾.

2.2 Interatomic potential between tool and workpiece

The interatomic potential between the tool and workpiece was assumed to be the two-body potential defined as Eq. (1) with parameters based on *ab-initio* molecular orbital (MO) calculations for the atom cluster in Fig. 2.

$$U(r_{ij}) = D[\exp\{-2\alpha(r_{ij} - r_0)\} - 2\exp\{-\alpha(r_{ij} - r_0)\}] + E \exp\{-\beta(r_{ij} - r_1)^2\} \quad (1)$$

In this atom cluster, a Cr or Ni atom was arranged at the hexagonal hollow site, (111), of the diamond structure. Hydrogen (H) atoms were also attached at the outside of the diamond structure for the electron density periodicity of a diamond or silicon. Bond energies between Cr and C (Cr-C), Cr and Si (Cr-Si), Ni and C (Ni-C), and Ni and Si (Ni-Si) atoms were calculated by using Gaussian 94⁽¹³⁾. In these MO calculations, the STO-3G basis set and the Hartree-Fock theory⁽¹³⁾ were used.

Figures 3(a) and 3(b) show the bond energies obtained in the MO calculations. The bond energy of Cr-C atoms have a peak of 0.5 to 1.0 eV at the atomic distance 0.3 nm, and that have a minimum peak of -0.1 to -1.0 eV at the atomic distance about 0.2 nm in Figs. 3(a). The shape of the bond energy curve of Ni-C atoms in Figs. 3(b) is similar to that of Cr-C atoms. These results indicate that adhesion of a Cr or Ni atom to C atoms is in need of the activated energy of

Fig. 2 Atom cluster model for molecular orbital calculations

0.5 to 1.0 eV. Bond energies of Cr-Si atoms and Ni-Si atoms do not have the minimum peak except the bond energy obtained from the Ni-Si₆H₉ cluster with the multiplicity 4. These energy curves are similar to a soft-core type potential. So, a Cr or Ni atom has more difficulty in adhering on Si atoms than C atoms. Table 2 lists the potential parameters determined by fitting MO results to Eq. (1). Potential parameters calculated by using the (Cr, Ni)-(C, Si)₆H₉ atom cluster with the multiplicity 4 will be applied to the

(a) Bond energy of Cr-C and Cr-Si atoms

(b) Bond energy of Ni-C and Ni-Si atoms

Fig. 3 Interatomic energy between tool and workpiece

Table 2 Potential parameters in two-body potential function

	D (eV)	α (1/Å)	r_0 (Å)	E (eV)	β (1/Å ²)	r_1 (Å)
Cr- C ₆ H ₉ m4	0.820	1.832	2.111	1.310	4.540	2.910
Cr- C ₆ H ₉ m2	0.238	2.280	2.230	0.890	4.941	2.950
Cr- Si ₆ H ₉ m4	0.014	2.083	2.610	0.015	4.929	3.141
Cr- Si ₆ H ₉ m2	0.310	2.882	2.620	0.691	2.540	2.701
Ni- C ₆ H ₉ m4	0.995	2.380	1.984	0.950	3.010	2.650
Ni- C ₆ H ₉ m2	0.290	2.270	2.201	1.150	2.850	2.850
Ni- Si ₆ H ₉ m4	0.450	4.170	2.480	-	-	-
Ni- Si ₆ H ₉ m2	0.040	2.460	3.060	-	-	-

Fig. 4 MD analyses of atomic scale indentation

interatomic potential between the tool and workpiece in 3D MD simulations.

3. Results and Discussions of Atomic Scale Indentation

3.1 Effect of material used for a tool on indentation mechanism

Three-dimensional MD simulations with three kinds of tool models examined the effect of material used for a tool on the indentation mechanism. Figures 4(a)–4(c) show atomic configurations in the indentation of the chromium with (a) the diamond; (b) the silicon; and (c) the DLC tool.

The plastic deformation of the chromium is observed in the indentation using the diamond tool for case (a), caused by the slip activity of the workpiece. However, the diamond tool is not deformed at all. As a result of this, the indentation mark on the top surface is generated during the process. The adhesion of a few Cr atoms to C atoms at the apex of the diamond tool is also observed while the tool is removed out of the workpiece. This is attributed to a larger adhesive energy between Cr and C atoms as shown in Figs. 3(a). The compressive deformation of

the silicon tool is seen during pushing the workpiece, and the tool atoms are disordered in Figs. 4(b). However, Cr atoms do not move except some Cr atom at the contact area between the tool and workpiece. This is caused by the lower elastic stiffness of the silicon tool than that of the chromium. So, to indent the chromium with the silicon tool is difficult owing to the plastic deformation of the tool. The DLC tool in Figs. 4(c) creates the large deformation and the indentation mark on the chromium. Some C atoms in the DLC tool are disordered during pulling the tool. The adhesion of C atoms in the DLC tool to the workpiece is also seen in this figure. The adhered atoms are released from the atomic connection by decreasing the adhesive force between tool atoms due to the kinetic energy increase during the indentation. So, the indentation of the chromium with the DLC tool probably led to wear at the apex of the tool.

In indentation simulations of the nickel with the diamond and DLC tools, some slip line and the indentation mark were observed on the workpiece, although the figures of the nickel were omitted here. These results were similar to the MD results of the chromium with the diamond and DLC tools.

Fig. 5 Load-penetration depth curves

However, in the indentation of the nickel with the silicon tool, the adhesion of the Ni atoms to the tool was observed. This is not corresponding to the MD result of the chromium with the silicon tool. This may be caused by increasing the attractive force between the tool and workpiece during the pulling the tool since the bond energy curve of Ni-Si atoms has the higher adhesive energy in the long range (Figs. 3(b)).

These MD results indicate that the deformation mechanism of the chromium and nickel during an atomic scale indentation depends on the material used for a tool. Using the tool with higher elastic stiffness produces the plastic deformation and indentation mark on the workpiece. The atomic adhesion during the indentation depends on the interatomic potential between the tool and workpiece.

3.2 Evaluation of Young's modulus in atomic scale indentation

Young's modulus of the workpiece was calculated by using a load-penetration curve in the atomic scale indentation simulation. Young's modulus E_r in an indentation was evaluated by the slope of the unloading curve using the following equation⁽¹⁴⁾,

$$E_r = \frac{1}{2} \sqrt{\frac{\pi}{A}} \frac{dP}{dh} \quad (2)$$

where dP/dh is the slope of the unloading curve and A the contact area.

Figures 5(a)-5(c) depict load-penetration depth curves in the atomic scale indentation simulations of the chromium with (a) the diamond; (b) the silicon; and (c) the DLC tools. The reaction force acting on the diamond tool increases with increasing the moving distance of the tool beyond 0.45 nm, but it turns to decrease below 0.7 nm for case (a). The point of reflection at the distance of 0.45 nm indicates the yield point of the chromium since some slip line on the workpiece was observed at this point (Figs. 4(a)). However, there is no point of inflection in the load-penetration depth curve, and the loading curve is in accord with the unloading curve in the indentation with the silicon tool for case (b). These mean that the

chromium does not yield during the indentation since the slip line and indentation mark were not seen clearly (Figs. 4(b)). The load-penetration depth curve in (c) is comparable to that in (a) except the slope of the loading and unloading curve. The smaller slope of the loading and unloading curve in (c) is ascribed to the sputtering and disorder of C atoms in DLC tool (Figs. 4(c)). Thus, the diamond tool is the most suitable tool for the atomic scale indentation among three kinds of tool used here since the plastic deformation and wear of the tool is not generated during the indentation.

Young's modulus E_r of the chromium was evaluated by the slope of the unloading curve in Fig. 5(a); as a consequence of this, the Young's modulus E_r in the MD analysis was 634 GPa. Young's modulus of a chromium in experiments is approximately known $E=248$ GPa⁽¹⁵⁾. So, the difference in Young's modulus between the MD analysis and experiments is about 256%. Young's modulus E_r of the nickel derived from the indentation simulation using the diamond tool was $E_r=721$ GPa, although the figure of load-penetration depth curve for the nickel was omitted here. The difference in Young's modulus between the MD analysis and experiments is over 300% since the Young's modulus in experiments is about $E=214$ GPa⁽¹⁵⁾. These large discrepancies between analyses and experiments are ascribed to; ① the effect of the restriction of workpiece atoms at the bottom surface on load-penetration depth curves; ② the difference in the indentation speed between MD analyses and experiments; ③ the effect of the surface energy generated in the indentation on elastic modulus; and so on. The restriction of atoms at the bottom surface (①) produces large repulsive forces between workpiece atoms during the indentation. Since the reaction force increases with increasing the repulsive force, the Young's modulus in the analyses was larger than that of experiments. The other reason, the effect of the surface energy on elastic modulus (③), has been explained by Hashimoto⁽¹⁶⁾, where it has been

demonstrated by using an analytical model of thin film under a tensile load P .

Assuming that λ is the elongation, l the length, b the width and h the thickness of film under the tensile load, the elastic strain energy and the surface energy of the film are, respectively,

$$U_e = \frac{E_e \lambda^2}{2l} b h, \quad (3)$$

$$U_s = 2\gamma_s \lambda (b + h). \quad (4)$$

Here, E_e is the Young's modulus including in no contribution of the surface energy and γ_s the surface energy per unit area.

The total energy of the film is equated as

$$U_{\text{total}} = U_e + U_s. \quad (5)$$

The total load is also defined by the following equation with Young's modulus E including in the contribution of the surface energy,

$$U_{\text{total}} = \frac{E\lambda}{2l} b h. \quad (6)$$

Combining Eqs. (3)–(6), the following equation is obtained,

$$E = E_e + \frac{4\gamma_s l}{\lambda} \left(\frac{1}{h} + \frac{1}{b} \right). \quad (7)$$

This equation indicates that the Young's modulus increases with decreasing the film thickness and it increases with increasing the surface energy.

The MD simulation models in this paper have a thin thickness on an atomic scale. The surface energy presumably increases during the indentation to produce a new surface at the indentation mark. Therefore, the larger Young's modulus in MD analyses was produced by an atomic scale thickness of workpiece and by the increase in the surface energy during the indentation.

4. Results and Discussions of Atomic Scale Cutting Process

4.1 Effect of material used for a tool on cutting mechanism

In order to reveal the effect of material used for a tool on the cutting mechanism and machinability of a metal workpiece, 3D MD cutting simulations were carried out for the chromium and nickel using the diamond and silicon pin tools. Here, to reduce the calculation time, the pin tools was pushed from a distant separation toward the workpiece surface with the indentation speed at 1 000 m/s before the cutting process.

Figures 6(a)–6(d) show atomic configurations during the cutting process of (a) the chromium using the diamond tool; (b) the chromium using the silicon tool; (c) the nickel using the diamond tool; and (d) the nickel using the silicon tool. Wedge shaped chips and side flow are formed around the diamond tool for

Fig. 6 MD analyses of atomic scale cutting process

case (a). Chips and side flow are also formed around the silicon tool for case (b). Comparing Figs. 6(a) with 6(b), the volume of chip and side flow in Figs. 6(b) is smaller than that in Figs. 6(a), caused by the plastic deformation of the silicon tool. In the cutting simulations of the nickel in Figs. 6(c) and 6(d), the chip and the side flow around the tool are not produced, but the burr is generated in front of both tools. There is the large difference in the chip formation between the chromium and nickel. This is caused by the influence of slip system in the workpieces on the chip formation.

Chromium single crystal has $\{110\}\langle 111 \rangle$ and $\{112\}\langle 111 \rangle$ slip systems, whereas nickel single crystal has a $\{111\}\langle 110 \rangle$ hexagonal slip system due to inelastic deformation at room temperature. The cutting direction of the chromium is not included in its slip system since the tools are moved in the $[001]$ direction on (110) surface in Figs. 6(a) and 6(b). In the cutting process of the chromium, the inconsistency in the direction between the cutting and slip system

Fig. 7 Atomic configurations of cross-section

resulted in the chip and side flow formation on the top surface. However, the tools used for the cutting of the nickel are moved in the $[110]$ direction on (111) surface in Fig. 6(c) and 6(d). The agreement between the cutting direction and the slip direction of nickel produced the burr in front of the tool.

Comparing Figs. 6(c) with 6(d), the burr produced by the silicon tool is smaller than that of the diamond tool. This results from wear of the silicon tool in Figs. 6(d). In this figure, silicon atoms falling off the tool is observed at the apex of the tool. The worn tool could not push the workpiece atoms fully in the cutting direction.

4.2 Machinability of workpiece in cutting process

For examining the depth of cut for the workpieces during the cutting process, the cross-section of workpieces is shown in Figs. 7(a) - 7(d). The depth of cut for both workpieces using the diamond tool increases with increasing the moving distance of the tool in the y -direction for case (a) and (c). This indicates that the normal load controlled condition in the process leads to creep deformation of the workpieces. However, the cutting process using the silicon tool does not make the deep groove for case (b)

and (d). Especially, the depth of cut for the nickel with the silicon tool is the shallowest among all the case. Nickel atoms at the 3 or 4 layers from the top are just removed owing to the deformation and wear of the tool during the cutting (Fig. 6(d)). These results suggest that a diamond is the most suitable tool material for the deep cutting of the nickel on an atomic scale.

The ratio of the tangential force to the normal force; F_t/F_n was measured during the cutting to study the machinability of the chromium and nickel on an atomic scale. Here, F_t is the tangential force acting on the tool and F_n the normal force. On a micro and millimeter scale, the increase in F_t/F_n results in the lower machinability and the decrease in F_t/F_n conversely the higher machinability. Figures 8(a) and 8(b) show the variation of the ratio F_t/F_n with the number of time steps in MD simulations. The ratio F_t/F_n of the chromium and nickel with the diamond tool is about 0.3 in Figs. 8(a). The ratio F_t/F_n of the chromium with the silicon tool is also approximately 0.3, whereas that of the nickel with the silicon tool is about 0.6 in Fig. 8(b). The cutting process of the nickel with the silicon tool indicates the lower machinability, caused by wear of the silicon tool as shown in Fig. 6(d). Wear, which means that silicon

Fig. 8 Ratio of tangential force to normal force; F_t/F_n

atoms fall off the tool, brings about the increasing contact area between the tool and workpiece. The tangential force increases with increasing the inter-atomic force between the tool and workpiece due to the larger contact area. Therefore, wear of the tool in the atomic scale cutting process results in the lower machinability.

4.3 Comparison of MD analyses with AFM experiments

Nano scale single-grid cutting experiments were carried out to study the depth of cut for the chromium and nickel on a nano scale. The depth of cut in nano scale experiments was compared with that in atomic scale experiments by MD simulations. Nano scale experiments for a chromium and nickel thin film were carried out using a silicon cantilever having about 10 nm tip radius. In this study, AFM (SEIKO INSTRUMENTS; SPA-300 HV) was used for the single-grid cutting tests. Table 3 lists the experimental condition including the scanning condition of the cantilever. Cutting tests were carried out at room temperature under the normal load of $16.7 \mu\text{N}$ at the cutting speed of $1.0 \mu\text{m/s}$. Although the experimental conditions are different from those in MD simulation, qualitative comparison of the experimental results with MD results contributes well to the understanding of the basic physical cutting process.

Figures 9(a) and 9(b) show AFM images of the chromium and nickel thin film. The depth of cut for

Table 3 Experimental conditions of cutting process with AFM

Chromium	AFM tip and Spring constant Normal load Tip move speed	Si, $k=17\text{N/m}$ $16.789 \mu\text{N}$ $1.0 \mu\text{m/s}$
Nickel	AFM tip and Spring constant Normal load Tip move speed	Si, $k=17\text{N/m}$ $16.740 \mu\text{N}$ $1.0 \mu\text{m/s}$
Scan condition		
Width : 50nm 100nm 150nm 200nm 250nm 300nm 350nm		
Scan direction		10nm 5 μm

the chromium is about 1.5 nm and the nickel less than 0.5 nm. These depths of cut are deeper than those in MD analyses. This may be caused by the difference between experimental and analytical conditions. There are differences in cutting speed, crystal orientation and the ratio of tool tip radius to cut depth between experiments and MD analyses. However, the cutting of the chromium with the silicon tool results in the deeper groove than that of the nickel for both experiments and MD analyses (Fig. 6(d) and 7(b)). Thus, the machinability in a nano scale cutting process can be predicted qualitatively by means of MD simulations.

5. Conclusions

1. The diamond and DLC tool produced the indentation mark on the top surface of the chromium and nickel, however the silicon tool did not make it owing to the tool deformation. The plastic deformation of the workpieces during an atomic scale indentation depends on the elastic stiffness of the tool.

2. Young's modulus of the chromium and nickel, which was evaluated by using load-penetration depth curves in MD simulations, was 250 - 300% larger than that in experiments. This could be qualitatively rationalized by the effect of the surface energy on the elastic modulus.

3. Using the diamond tool performed the deep cutting of the chromium and nickel whereas using the silicon tool did not, caused by the plastic deformation and wear of the silicon tool. The machinability of the nickel with the silicon tool was the lowest among all the case since the ratio F_t/F_n during the cutting resulted in the highest value. Diamond is a suitable tool material for the deep cutting on an atomic scale.

(a) Chromium

(b) Nickel

Fig. 9 AFM images in direct cutting process

4. The depth of cut in nano scale cutting was similar to that in atomic-scale cutting, resulting from the comparison of experimental results with MD results. Thus, it seems that the machinability in nano scale cutting can be predicted qualitatively by means of MD simulations.

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