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Original Citation

Oluwajobi, Akinjide O. and Chen, Xun (2010) The effect of tool geometry on rubbing and ploughing phenomena in nano abrasive machining. In: Future Technologies in Computing and Engineering: Proceedings of Computing and Engineering Annual Researchers' Conference 2010: CEARC'10. University of Huddersfield, Huddersfield, pp. 160-165. ISBN 9781862180932

THE EFFECT OF TOOL GEOMETRY ON RUBBING AND PLOUGHING PHENOMENA IN NANO ABRASIVE MACHINING

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ABSTRACT

The effects of cutting edge shapes on the phenomena of rubbing and ploughing in nano-abrasive machining were investigated. The shapes under investigation include flat, spherical and trapezoidal shapes. The tool with the flat end geometry shows a fast initiation of ploughing, because it has the largest surface area to engage more atoms. It doesn't show rubbing phenomenon at the (initial) depth of cut of 0.5 Angstroms. The tool with the trapezoidal end has the lowest average cutting force and the tool with the flat end has the highest average cutting force.

Keywords tool geometry, rubbing, ploughing, molecular dynamics, abrasive machining

1 INTRODUCTION

The selection of effective and optimal machining parameters is a major challenge for the manufacturing industries. The tool-work interactions may be affected by many process parameters including depth of cut, cutting speed, feed rate, cutting tool geometry et cetera. Proper selection of these parameters is critical in material removal processes. With the trend towards miniaturization and the development of ultra–precision processes which can achieve excellent surface finish at nanometre level, there is a need for in-depth study of the effects of these parameters. Unlike in conventional cutting processes, where the undeformed chip thickness is significant compared to the cutting edge radius; in nano-abrasive machining, the undeformed chip thickness is very small. Therefore, the cutting edge effects cannot be ignored (Komanduri et al (1998)). Currently, it is very difficult to observe the diverse microscopic physical phenomena occurring in nanometric machining through experiments. The use of Molecular Dynamics (MD) simulation may prove to be an effective way for the analysis and prediction of machining processes at the nanometre scale. This research studies the effect of tool edge geometry in nano-abrasive machining using the MD. The MD method was initiated in the late 1950s at Lawrence Radiation Laboratory in the US by Alder and Wainwright in the study of statistical mechanics (Alder and Wainwright (1959)). Since then, the use of the MD simulation method has spread from Physics to Materials Science and now to Mechanical Engineering. The MD method can improve our understanding of nanometric processes and subsequently give helpful insights into phenomena that are otherwise intractable to investigate experimentally. Initially, the method was used extensively to model indentation and cutting. In 1991, Belak and Stowers first applied the MD to abrasive processes (Belak and Stowers (1991)) and Rentsch and Inasaki's study later presented the first results of simulations targeted on the pile-up phenomenon in abrasive machining (Rentsch and Inasaki (1994)). In the field of nanometric cutting, Belak pioneered work on the study of cutting copper with a diamond tool (Belak and Stowers (1999)).

2 FUNDAMENTALS OF MD AND EXAMPLES OF MD

Molecular dynamics (MD) is a computer simulation technique used in the study of the motions of a set of particles – atoms. The technique works by following the time evolution of a set of interacting atoms while integrating the equations of their motion. The MD is deterministic. Once the positions, velocities and accelerations of the particles are known, the state of the system can be predicted. The method is based on statistical mechanics – a way to obtain a set of configurations distributed according to some statistical distribution functions (Ercolessi (1997)). The foundation of MD simulation is based on Newton's second law of motion. It consists of the numerical step-by-step solutions of the classical equations of motion. For a set of N atoms,

$$F_i = m_i a_i \qquad (1)$$

Where m_i is the mass of atom *i*, $a_i = \frac{d^2 r_i}{dt^2}$, the acceleration of the atom *i* and F_i is the force acting on atom *i*. (The forces are usually obtained as the gradient of a potential energy function).

Basuray et al (1977) analyzed the transition from ploughing to cutting during machining with blunt tools. They observed that when machining at small depths of cut, metal flow near a rounded tool edge becomes important. Also, when a blunt tool approaches the workpiece, the material is compressed and is either ploughed under the flank face of the tool or becomes separated from the bulk material in the form of a chip (see figure 1). They concluded that there exists a critical depth of cut during machining with blunt tools and the neutral point of angle corresponding to this depth is 37.6^o. (Where the neutral point angle is angle θ in figure 1b.) Fang et al (2003) carried out systematic study of various types of tool geometry (with diameters of 0.1mm) in micromachining (see figure 2). Their experimental results show that the tool tip rigidity of the semi circular-based (D-type) end mills is much higher than that of the 2-flute (commercial type) end mills and the machining quality with D-type tools is better than that of the triangle-based end. Komanduri et al (1998) investigated the effect of tool geometry in nanometric cutting. MD studies were conducted with various tool edge radii (1.81-21.72nm) and depths of cut (0.362-2.172nm) at constant ratios (0.1, 0.2, 0.3) of the depth of cut to the tool edge radius (d/r). They considered indentation sliding to simulate the ultraprecision machining, grinding and abrasion (see figure 3). Results showed that with tools of different radii, the cutting force increase with depth of cut, independent of the (d/r) ratio. Also, the specify energy increased rapidly with decrease in depth of cut. They proposed that for grinding of ductile materials, the appropriate model would be machining using tools of either large radii relative to the depth of cut or large negative rake angle. Komanduri et al study was focused on pointed tools with various radii, but abrasive grains could be of different and complex shapes, which require that various tool end shapes should be investigated for practical realism.

3 THE MD MODEL FOR THE SIMULATIONS

Morse potential (Morse (1929)) was used in this investigation. The Morse potential can be expressed as

$$V_{ij} = D\{\exp[-2\alpha(r_{ij} - r_e)] - 2\exp[-\alpha(r_{ij} - r_e]\} \qquad (2)$$

Where r_{ij} and r_e are instantaneous and equilibrium distances between atoms *i* and *j* respectively, α and D are constants determined on the basis of the physical properties of the material

Table 1 shows the simulation conditions applied in this research. In the investigation, the workpiece consists of 16000 copper atoms with FCC lattice. It includes 3 types of atoms namely; boundary atoms, thermostat atoms and Newtonian atoms. The boundary atoms are kept fixed to reduce edge effects. The thermostat atoms conduct the heat generated during the cutting process out of the workpiece and the Newtonian atoms obey the Newton's equation of motion. The cutting tools consist of carbon atoms with diamond lattice structure. The different cutting tools are modelled as rigid bodies.

The atomic interactions in the simulation are the following, namely;
Cu-Cu : interactions between copper atoms
Cu-C : interactions between copper atoms and diamond atoms
C-C : interactions between the diamond atoms (treated as rigid)
The LAMMPS MD software (Plimpton (1995)) was used for the simulations.

Tool Geometries

Three tools shapes investigated in this study are shown in figure 4, namely; the tools with spherical, flat and trapezoidal ends. The parameters of Morse potential used in the simulation are given as follows:

For Cu-Cu interactions: (Girifalco (1959), Pei et al (2006))

$D = 0.3429eV,\ \alpha = 0.13588(nm)^{-1},\ r_e = 0.2866nm$

For Cu-C interactions: (Hwang et al (2004))

$D = 0.087eV,\ \alpha = 0.17(nm)^{-1},\ r_e = 0.22nm$

The summary of the results are given in Table 2. The flat end tool induces ploughing when the depth of cut is only 0.5 angstrom, while the trapezoidal end tool requires more depth of cut to plough materials. This is because the flat edge constrains more atoms and squeezes them upwards. For the depth of cut of 5 angstroms; the ratios of the depth of cut to tool radius (d/r) are 0.26, 0.41 and 0.68 for the flat edge, the spherical edge and the trapezoidal edge respectively.

4 RESULTS AND DISCUSSIONS

The cutting forces for the various tool geometries are shown in figures 5 to 7. The average cutting force (F_x) for the flat end, spherical end and trapezoidal end are -1.47E-13N, -3.23E-13N and -3.92E-13N respectively. The cutting force (F_x) is highest for flat end and lowest for the trapezoidal end. The force intensities at depth of cut of 5 angstroms are -0.52N/mm^2, -1.15N/mm^2 and -3.25N/mm^2 for the flat, spherical and trapezoidal tools respectively. The force intensity is also highest for the flat end and lowest for the trapezoidal end. The tools in increasing order of sharpness are the following, namely; the tool with the flat end (least sharp), the tool with the spherical end and the tool with the trapezoidal end (sharpest). The tools show the initiation of ploughing in that order. The tool with the flat end geometry shows a fast initiation of ploughing, because it has the largest surface area to engage more atoms.

5 CONCLUSIONS

Simulation results demonstrated the ploughing phenomenon in nanomaterial removal process and this depends on the cutting edge shape. The flat cutting edge can induce ploughing with lowest depth of cut. The tool with the trapezoidal end has the lowest average cutting force and the tool with the flat end has the highest average cutting force. It can be noted, that the sharpest cutting edge doesn’t necessarily indicate the most effective cutting edge for material removal on the nanoscale. The simulations were carried out with zero degree rake angles, so further studies would investigate the effect of different rake angles on the different tool geometry.

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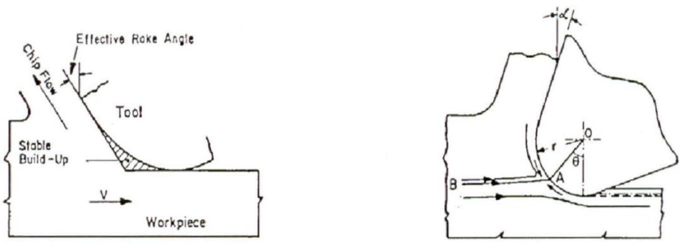


(a) (b)

Figure 1: (a) A stable built-up edge during machining with blunt tools, (b) The metal flow around a rounded tool edge (Basuray et al (1977))

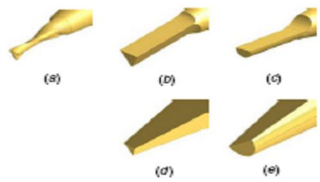
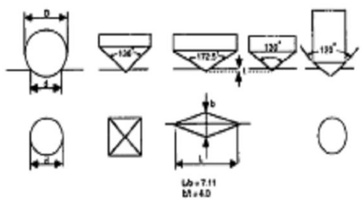
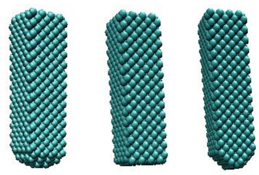


Figure 2: Various types of end-mills in micromachining.
(a) Two-flute end-mills, (b) Triangular-type end-mills with a straight body, (c) D-type end-mills with a straight body, (d) triangular-type end-mills with a tapered body and (e) D-type end-mills with a tapered body (Fang et al (2003))



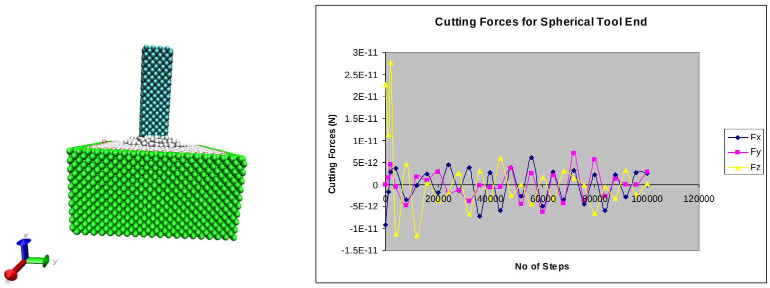
(a) (b) (c) (d)

Figure 3: Geometry of spherical, Vicker's, knoop and Diamond indentation. (a) Spherical indenter, (b) Vickers diamond pyramid indenter, (c) Knoop diamond pyramid indenter and (d) Diamond cone indenter (Komanduri et al (1998))



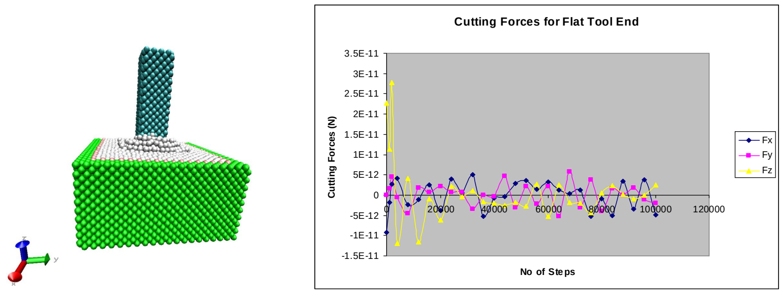
(a) (b) (c)

Figure 4: Different tool geometries; (a) Tool with spherical end, (b) Tool with flat end, (c)Tool with trapezoidal end,



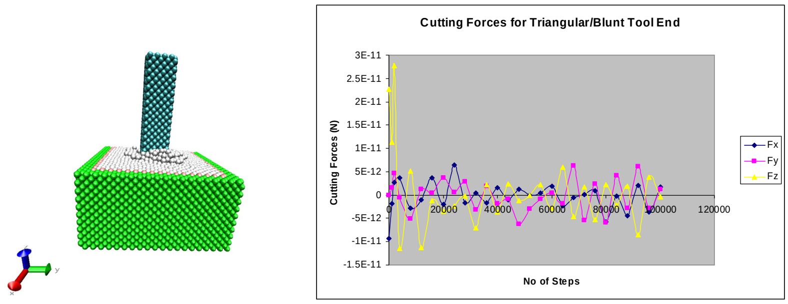
(a) (b)

Figure 5: (a) Simulation with spherical end tool, (b) Cutting forces for depth of cut of 5 Angstroms



(a) (b)

Figure 6: (a) Simulation with flat end tool, (b) Cutting forces for depth of cut of 5 Angstroms



(a) (b)

Figure 7: (a) Simulation with trapezoidal end tool, (b) Cutting forces for depth of cut of 5 Angstroms

Parameters	**Values**
Bulk Temperature	*293 K*
Cutting Direction	*[100]- Along the x-axis*
Cutting Speed	*150m/s*
Cutting Depth	*0.5nm*
Time Step	*0.3fs*
Run	*100000steps*

Table 1: MD simulation parameters

Depth of Cut (Angs)	**Flat End**	**Spherical End**	**Trapezoidal End**
0.5	Displacement of a lot of atoms/ ploughing	Displacement of few atoms	Rubbing
1.0	Ploughing with 1 layer of atoms	Displacement of more atoms	Displacement of few atoms
1.5	Ploughing with 1 layer of atoms	Displacement of more atoms/ploughing	Displacement of more atoms
2.0	Ploughing with 1 layer of atoms	Ploughing with 1 layer of atoms	Displacement of more atoms
2.5	Ploughing with 2 layer of atoms	Ploughing with 1 layer of atoms	Displacement of more atoms/ploughing
3.0	Ploughing with 2 layer of atoms	Ploughing with 1 layer of atoms	Ploughing with 1 layer of atoms
3.5	Ploughing with 2 layer of atoms	Ploughing with 1 layer of atoms	Ploughing with 1 layer of atoms
4.0	Ploughing with 3 layer of atoms	Ploughing with 2 layer of atoms	Ploughing with 1 to 2 layer of atoms
4.5	Ploughing with 3 layer of atoms	Ploughing with 2 layer of atoms	Ploughing with 2 layer of atoms
5.0	Ploughing with 4 layer of atoms	Ploughing with 3 layer of atoms	Ploughing with 3 layer of atoms

Table 2: Summary on various tool geometries (observed phenomena)