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THE EFFECT OF THE VARIATION OF TOOL END GEOMETRY ON MATERIAL REMOVAL MECHANISMS IN NANOMACHINING

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ABSTRACT

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. The effect of different geometric end shapes on the phenomena of rubbing and ploughing in nanomachining was investigated by using the Molecular Dynamics (MD) simulations. The shapes used were flat, pointed, spherical and trapezoidal. 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, the tool with the trapezoidal end and the tool with the pointed 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. The total energy is lowest for the tool with the pointed end and highest for the tool with the flat end. All the tools clearly show the phenomena of rubbing and ploughing in the depth of cut range of 0.05 to 0.5 nm. The tool with the pointed end has the lowest average cutting force and the tool with the flat end has the highest average cutting force. It is important to note that in nanomachining the tool with sharpest end may not necessarily cause the greatest material removal! The different tool ends may be suitable for different semiconductor and metal machining applications.

Keywords: Tool Geometry, Material Removal Mechanism, Molecular Dynamics Simulation

1. INTRODUCTION

Metal removal technologies play essential roles in modern manufacturing. As the scale reduces to the nanometre length and the chips removed are very small, as in highly precise machine parts, the mechanism of material removal is not fully understood. Unlike in conventional cutting processes, where the undeformed chip thickness is significant compared to the cutting edge radius, in nanomachining, the undeformed chip thickness is very small. Therefore, the cutting edge effects cannot be ignored [1]. 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 [2]. 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. In the field of nanometric cutting, Belak pioneered work on the study of cutting copper with a diamond tool [3]. Initially, the method was used extensively to model indentation and cutting. In 1991, Belak and Stowers first applied the MD to abrasive processes [4] and Rentsch and Inasaki's study later presented the first results of simulations targeted on the pile-up phenomenon in abrasive machining [5]. Komanduri et al [1] 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, and 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. 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.

2. THE MD MODEL FOR THE SIMULATIONS

In the investigation, the workpiece consists of 16000 copper atoms with Face Centred Cubic (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 and have varying number of atoms because of the different shapes. The flat end tool consists of 1824 atoms, the pointed end tool consists of 1936 atoms, the spherical end tool consists of 1839 atoms and the trapezoidal end tool consists of 1924 atoms. The different cutting tools were modelled as deformable, non-rigid bodies. The LAMMPS MD software [6] was used for the simulations and the Visual Molecular Dynamics (VMD) [7] was used for the visualization of the results.

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

The Embedded Atom Method (EAM) potential was used for the Cu-Cu interactions and the Lennard-Jones (LJ) potential was used for the Cu-C interactions. All the C-C (tool atoms) interactions were modelled by using the Tersoff potential.

The parameters used for the Cu-Cu interactions are given in [8] and the parameters used for the Cu-C interfaces are a slight variation of the values given in [9], with a cut-off distance of 2.5 Angstroms;

$\varepsilon = 0.4096eV$, $\sigma = 2.338\, Angstroms$

For the C-C interactions, the Tersoff potential parameters used are the following [10, 11];

A(eV) = 1.3936×10^{3}; B(eV) = 3.467×10^{2}; $\lambda_1(nm^{-1})$ = 34.879; $\lambda_2(nm^{-1})$ = 22.119;
α = 0.0; β = 1.5724×10^{-7}; n = 7.2751×10^{-1}; p = 3.8049×10^{4}; q = 4.384;
h = -5.7058×10^{-1}; $\lambda_3(nm^{-1})$ = 22.119; R (nm) = 0.18; D(nm) = 0.02.

Where R and D are cutoff parameters; $A, B, \lambda_1, \lambda_2, \lambda_3, \alpha, \beta, n, p, q, h$ are fitting parameters of the Tersoff potential.

Different Tool Geometries [12]

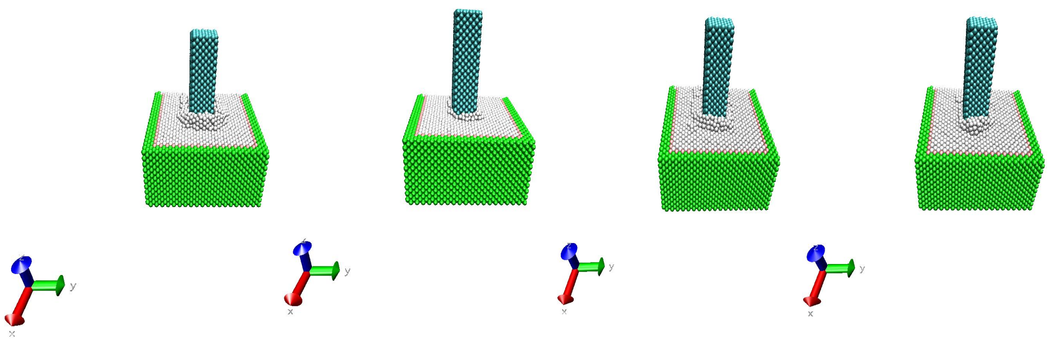
The tools shapes investigated in this study are shown in Figure 1, namely; the tools with spherical, flat, trapezoidal and pointed ends. Also, the corresponding simulations for the depth of cut of 0.5nm are shown in Figure 2.

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

Figure 1: Different tool geometries; (a) Tool with flat end (b) Tool with pointed end, (c) Tool with spherical end, (d) Tool with trapezoidal end

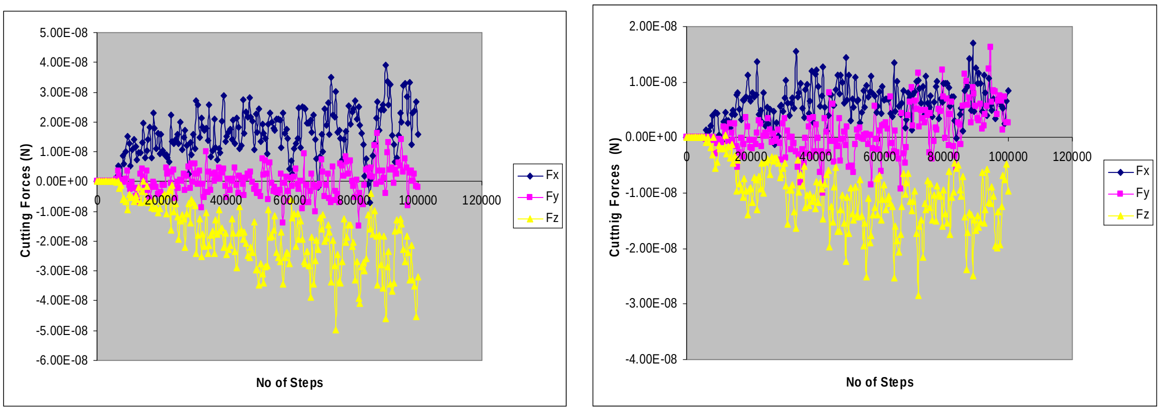
3. SIMULATION RESULTS

The corresponding simulations for the depth of cut of 0.5nm are shown in Figure 2 for the different tools showing the various removal of atoms.



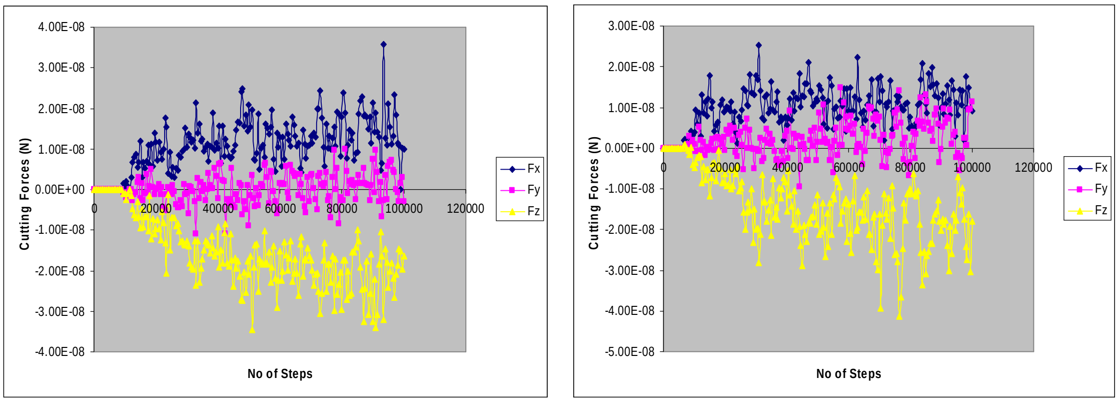
(a) (b) (c) (d)

Figure 2: Simulation for Depth of Cut 0.5nm: (a) Tool with flat end (b) Tool with pointed end, (c) Tool with spherical end, (d) Tool with trapezoidal end



(a) (b)

Figure 3: Cutting Forces for Depth of Cut – 0.5nm (a) Flat End Tool (b) Pointed End Tool



(a) (b)

Figure 4: Cutting Forces for Depth of Cut – 0.5nm (a) Spherical End Tool (b) Trapezoidal End Tool

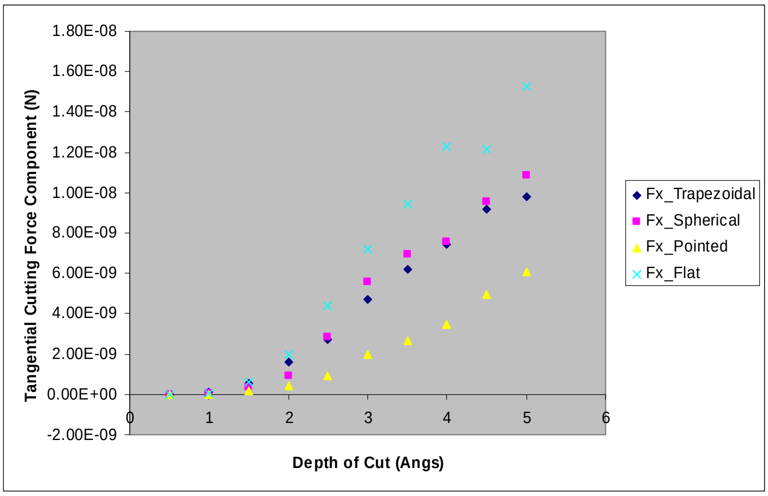


Figure 5: Variation of the Average Tangential Cutting Force with Depth of Cut for the Different Tool Ends

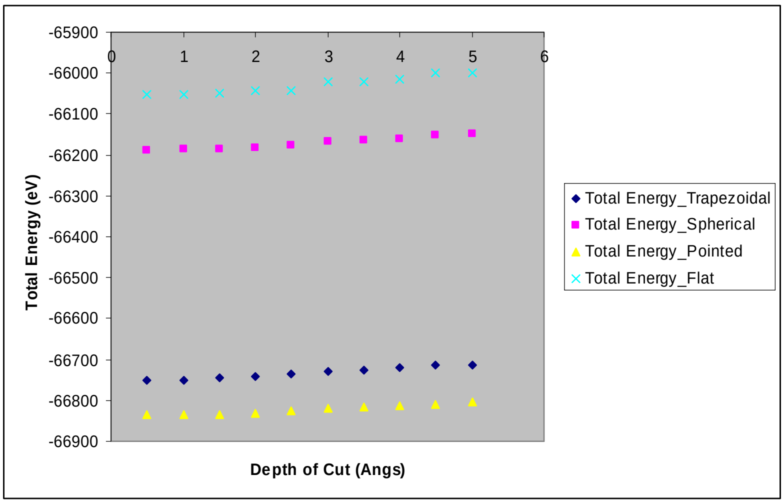


Figure 6: Variation of the Total Energy with Depth of Cut for the Different Tool Ends

4. DISCUSSIONS

Figures 3 and 4 show the cutting forces for all the four tool ends, for the depth of cut of 0.5nm. The summary of the results on rubbing and ploughing are presented in Table 1. Rubbing phenomena are observed in all the four geometries up to the depth of cut of 0.25nm. Also, for all the tools, ploughing initiates at the depth of cut of 0.3nm, but the tool with the flat end geometry shows a faster initiation of ploughing with three layers of atoms, because it has the largest surface area to engage more atoms.

Figure 5 shows the variation of the tangential cutting force component, Fx with depth of cut for all the tools. It can be observed that the tool with the pointed end has the lowest cutting force and it is highest for flat 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, the tool with the trapezoidal end and the tool with the pointed 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. Figure 6 shows the variation of the total energy with depth of cut for all the tools. The total energy is lowest for the tool with the pointed end and highest for the tool with the flat end.

Table 1. Summary on Various Tool Geometries (Observed Phenomena)

Depth of Cut (nm)	Flat Tool End	Pointed Tool End	Spherical Tool End	Trapezoidal Tool End
0.05	Rubbing	Rubbing	Rubbing	Rubbing
0.1	Rubbing	Rubbing	Rubbing	Rubbing
0.15	Rubbing	Rubbing	Rubbing	Rubbing
0.2	Rubbing	Rubbing	Rubbing	Rubbing
0.25	Rubbing	Rubbing	Rubbing	Rubbing
0.3	Ploughing with three layers of atoms	A slight initiation of ploughing with a number of side atoms	Ploughing with one layer of atoms	Ploughing with one layer of atoms
0.35	Ploughing with three layers of atoms	Ploughing with some few atoms	Ploughing with two layer of atoms	Ploughing with one layer of atoms
0.4	Ploughing with three layers of atoms	Ploughing with some few atoms	Ploughing with two layer of atoms	Ploughing with two layer of atoms
0.45	Ploughing with Five layers of atoms	Ploughing with some more side atoms	Ploughing with two layers of atoms	Ploughing with three layers of atoms
0.5	Ploughing with Four layers of atoms	Ploughing with two layers of atoms	Ploughing with three layers of atoms	Ploughing with three layers of atoms

5. CONCLUSION

All the tools clearly show the phenomena of rubbing and ploughing in the depth of cut range of 0.05 to 0.5 nm. The tool with the pointed end has the lowest average cutting force and the tool with the flat end has the highest average cutting force. It is important to note that in nanomachining the tool with the sharpest end may not necessarily cause the greatest material removal! The different tool ends may be suitable for different metal machining applications.

6. REFERENCES

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