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ON MINIMUM DEPTH CUT IN NANOMACHINING

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ABSTRACT

The concept of Minimum Depth of Cut (MDC) is that the depth of cut must be over a certain critical thickness before any chip is formed. It is actually a major limiting factor on achievable accuracy in nanomachining, because the generated surface roughness is primarily attributed to the ploughing process when the uncut chip thickness is less than the MDC. This paper presents an analysis of a cutting process where a sharp pointed diamond tool with an edge radius of an atom acts on a crystalline copper workpiece. From the molecular dynamics (MD) simulation results, the phenomena of rubbing, ploughing and cutting were observed. The formation of chip occurred from the depth of cut thickness of 30.0 Å (3nm).

Keywords: Minimum Depth of Cut, Nanomachining

1 INTRODUCTION

The Minimum Depth of Cut (MDC) is defined as the minimum undeformed chip thickness that can be removed stably from a work surface at a cutting edge under perfect performance of a machine tool (Ikawa et al 1992). The concept of MDC is that the depth of cut must be over a certain critical thickness before any chip is formed. This phenomenon of MDC leads to a rising of slipping forces, burr formation and surface roughness (Ducobu et al 2009). Conventionally, the tool-workpiece material interface has been considered to be homogeneous and continuum mechanics are used in the analysis of the MDC. In nanomachining, analysis is based on discrete atoms whose interactions are governed by appropriate intermolecular potentials. The understanding and the accurate prediction of the MDC is very crucial in improving the ultra-precision metal removal technologies, as this would assist in the selection of appropriate machining conditions and optimal geometry design.

The significance of MDC has been a topic of research in metal cutting mechanics since the last century (Sokolowski 1955 and Brammertz 1961). Subsequently, there has been a lot of focus on the estimation of the MDC in micromachining. The relationship between cutting edge sharpness and the MDC was analyzed by Yuan et al 1996. They obtained MDC in the range of 0.05µm – 0.2µm for diamond tool cutting edge radii of 0.2µm – 0.6µm, using the equation (1);

$$\lambda_{\min} = r \left(1 - \frac{F_y + \mu F_x}{\sqrt{(F_x^2 + F_y^2)(1 + \mu^2)}} \right) \quad (1)$$

Where λ_{\min} is the MDC, r is the tool edge radius, F_x is the horizontal force, F_y is the vertical force and μ is the coefficient of friction.

Weule et al 2001 observed the MDC effect in micromilling process. The cutting experiments were carried out with tungsten carbide tools edge radii of around $5\mu\text{m}$, on SAE 1045 steel. The minimum chip thickness to edge radius ratio of 0.293 was obtained for micromachining.

A Finite Element (FE) model has been used to determine the MDC for the single-phase ferrite and pearlite phases at micromilling length scales (Vogler et al 2004a). The edge radii of $2\mu\text{m}$ and $7\mu\text{m}$ with a range of chip thickness of $0.1\mu\text{m}$ - $3\mu\text{m}$ were used. Results showed that the MDC value for ferrite is greater than for pearlite. Similarly, the effect of MDC on the cutting forces in micromilling was studied by (Vogler et al 2004b). It was concluded that the MDC requires two separate force models to be able to handle the situations of chip and non-chip formations. Also, it was found that the frequency spectra of the forces contain a component that is a subharmonic of the tooth-passing frequency at feed rates less than the MDC and appears as a stepping behaviour of the forces in the time domain.

Son et al 2005 proposed an ultra precision cutting model in which the tool edge radius and the friction coefficient are the major factors for the determination of the MDC with a continuous chip. The model was based on equation (2).

$$\lambda_{\min} = r \left(1 - \cos \left(\frac{\pi}{4} - \frac{\beta}{2} \right) \right) \quad (2)$$

Where λ_{\min} is the MDC, r is the tool edge radius and β is the friction angle between a tool and an uncut workpiece passed under the tool.

From the model, MDC obtained for aluminium, brass and Oxygen Free High Conductive (OFHC) copper were in the range $0.09\mu\text{m}$ - $0.12\mu\text{m}$. It was noted that surface quality was best and continuous chip was generated when cutting was at the minimum thickness. Liu et al 2006 developed an analytical model, based on the molecular-mechanical theory of friction, for the prediction of the normalized chip thickness (λ_n) for 1030 steel and Al6082-T6. The λ_n was defined as the ratio of the minimum chip thickness to the tool edge radius. The model was based on the Kragelsky-Drujuanov equation (Kragelsky et al 1982) (see equation 3).

$$\lambda_n = \frac{h_{\min}}{r_n} = \frac{tc_{\min}}{r_e} = 0.5 - \frac{\tau_a}{\sigma} \quad (3)$$

Where h_{\min} is the limiting depth of penetration of an indenter and it is equivalent to the minimum chip thickness tc_{\min} in micromachining, r_n is the radius of indenter and it is equivalent to the rounded cutting edge radius r_e , σ is the effective flow stress of strain-hardened bulk material, τ_a is the shear strength of the adhesive junction of chip/tool interface.

It was found that λ_n increases as the cutting velocity and tool edge radius increases when machining carbon steels. On the other hand, the λ_n remains constant over a range of cutting velocities and tool radii, when machining Al6082-T6.

On nanomachining, the Ikawa group in Osaka did a lot of work on the MDC, with the aim of achieving machining nanometric accuracy (Ikawa et al 1991, Ikawa et al 1992 and Shimada et al 1993). A 2-D simulation of copper atoms machined by a diamond tool, with edge radius of 5 to 10nm was used for the MD studies. Using the Morse potential and a cutting speed of 200m/s, initial stage of chip removal was observed for depth cut larger than 0.3nm and the MDC increased to 0.6nm with a larger edge radius of 10nm. From their studies, they proposed that the MDC in nanocutting would be about 0.5nm to 1nm, (which is 0.05 to 0.1 of the edge radius).

The different approaches for the determination of the MDC include the Molecular Dynamics approach (Shimada et al 1993), experimentation (Yuan et al 1996), FEM approach (Vogler et al 2004) and analytical approach (Liu et al 2006). The experimental method for the estimation of the MDC would be very tedious and expensive (it is not feasible presently for nanometric cutting) and the accuracy will be strongly affected by experimental uncertainties (Liu et al 2006). The Finite Element Method (FEM) approach is also not suitable, because nano machining phenomena take place in a small limited region (tool – workpiece interface), usually the surfaces containing few atoms or layers of atoms and it is not continuous as assumed by continuum mechanics. Also, the analytical approach to nanomachining would be very difficult, as the basics would be in quantum mechanics. The Molecular Dynamics (MD) lends itself to the solution of this problem, as the dynamics of the material removal process can be modelled in the simulation.

2 MD SIMULATION METHODOLOGY

The workpiece consists of 16000 atoms with perfect FCC copper lattice. It includes 3 kinds 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 tool consists of 912 atoms with perfect diamond lattice structure, and it is modelled as a rigid body. 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)

Parameters Used:

The Morse Potential was used for the simulation (see equation 4)

$$V_{ij} = D\{\exp[-2\alpha(r_{ij} - r_e)] - 2\exp[-\alpha(r_{ij} - r_e)]\} \quad (4)$$

For Cu-Cu interactions: (Girifalco and Weizer(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)

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

Other parameters used was viz; Bulk Temperature -293 K, Cutting Direction-[100], Cutting Speed - 150m/s, Time Step - 0.3fs, Run - 100000steps, Cut-off distance - 0.64nm and LAMMPS MD software (Plimpton 1995) was used for the simulations. A sharp pointed diamond tool with an edge radius of an atom (2.45 Å) was used on the crystalline copper atoms workpiece. MD computational experiments were conducted, by using the above parameters and then varying the depth of cut from a base point of 0.0Å. Initially, the increment of 0.1 Å depth of cut was used and then 0.5 Å, 5 Å and 10 Å.

3 RESULTS AND DISCUSSIONS

MD simulation results show that from the depth cut of 0.1 to 1.5Å, rubbing phenomena are observed; where no atoms are moved from their original positions after cutter passes them. Ploughing, referred to atoms been displaced permanently, initiates from around 3Å depth of cut, with a transition phase between 1.6Å to 2.5Å. With the onset of ploughing, the pile-up of atoms begins from one atom up to seven layers of atoms. The cutting phenomena (or chip formation) start to occur around 30Å (See Table 1). The above phenomena are shown in Figures 1-4, with the associated cutting forces. As the cutting depth increases,

the variation of the cutting forces is shown in Figure 5. It can be seen that the cutting force increases gradually with the depth of cut, albeit the variation of the force is significant. This is because the force acting on the individual atoms depends on their positions and velocities in the simulation.

Table 1: Summary - Minimum Depth Cut

Depth of cut (Å, angstroms)	Build-up/Pile-up Phenomena	Comments
0.0 – 1.5	None	Rubbing/Elastic Deformation
1.6 - 2.0	None	Rubbing/some few atoms were displaced-removed from the edge surface
2.5	None	Rubbing/ploughing - some atoms were displaced
3.0	One atom	Ploughing
3.5	Few atoms	Ploughing
4.0 – 4.5	One layer of atoms	Ploughing
5.0	Two layers of atoms	Ploughing
10.0	Four layers of atoms	Ploughing
15.0	Five layers of atoms	Ploughing
20.0	Seven layers of atoms	Ploughing
30.0	Eight layers of atoms	Ploughing/cutting
35.0	Nine layers of atoms	Cutting

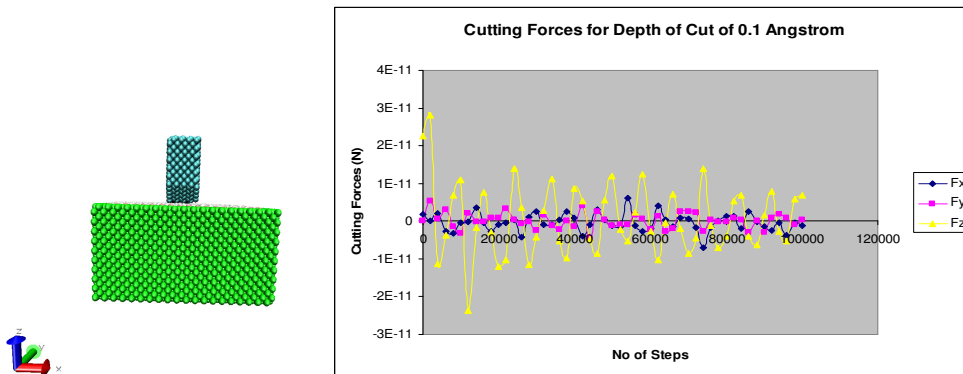


Figure 1: Depth of Cut and Cutting Forces for Depth of Cut - 0.1 Å

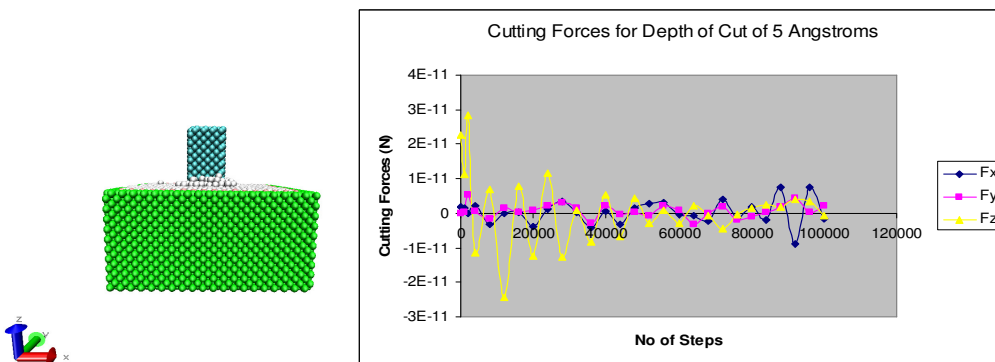


Figure 2: Depth of Cut and Cutting Forces for Depth of Cut – 5.0 Å

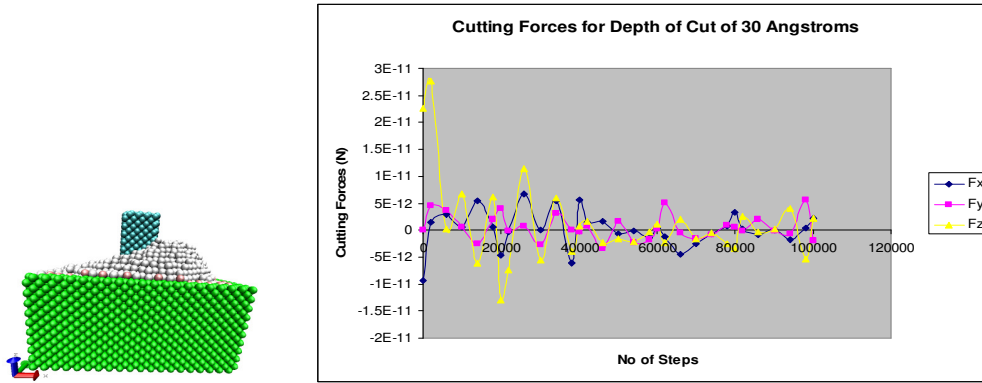


Figure 3: Depth of Cut and Cutting Forces for Depth of Cut – 30.0 Å

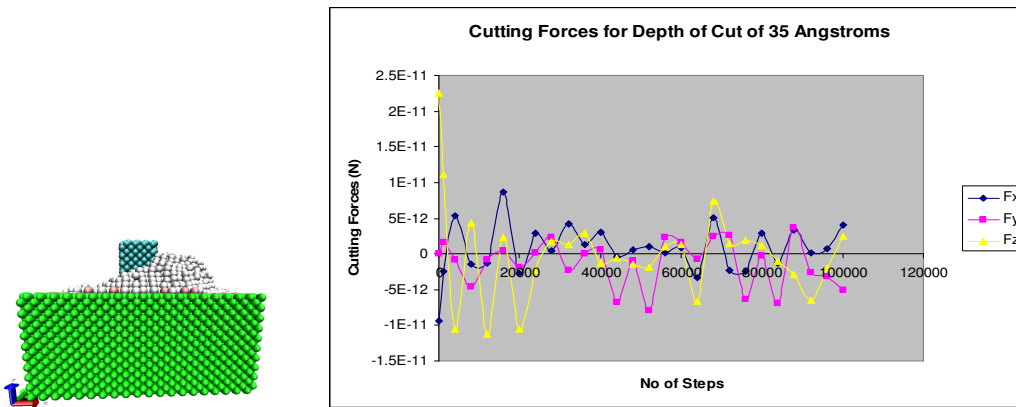


Figure 4: Depth of Cut and Cutting Forces for Depth of Cut – 35.0 Å

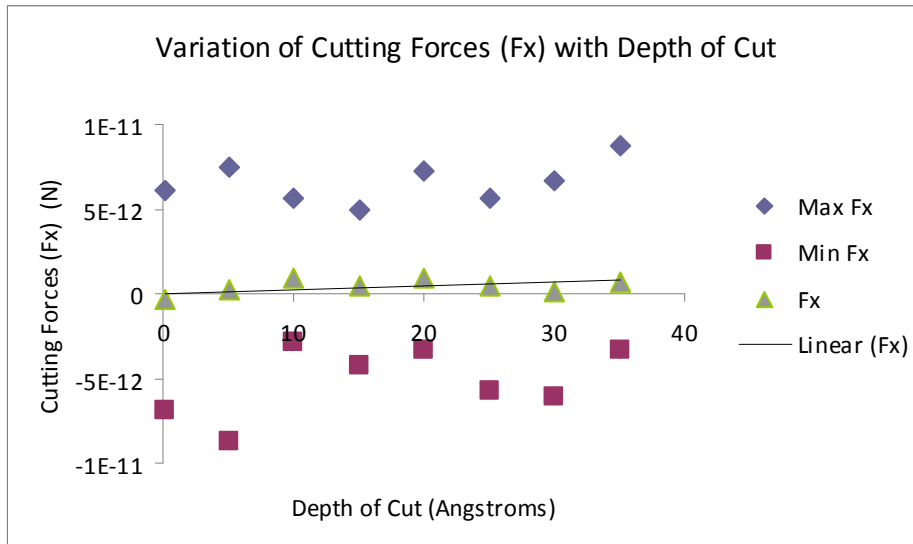


Figure 5: The Variation of Cutting Forces with Depth of Cut

4 CONCLUSION

From the MD simulation results, the phenomena of rubbing, ploughing and cutting are observed, with the formation of chips occurring from the depth of cut thickness of 30.0 Å (3nm). So it can be suggested that the extreme accuracy attainable or MDC for copper atoms workpiece, machined with extremely sharp diamond tool with edge radius of 2.45Å is around 30.0 Å to 35 Å (3-3.5nm).

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