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Multi-Pass Nanometric Machining Simulation using the Molecular Dynamics (MD)

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Abstract

The multi-pass nanometric machining of copper with diamond tool was carried out using the Molecular Dynamics (MD) simulation. The copper-copper interactions were modelled by the EAM potential and the copper-diamond interactions were modelled by the Morse potential. The diamond tool was modelled as a deformable body and the Tersoff potential was applied for the carbon-carbon interactions. It was observed that the average tangential and the normal components of the cutting forces reduced in the consecutive cutting passes. Also, the lateral force components are affected by atomic vibrations and the cross sectional area during the cutting process.

Introduction

The trend towards miniaturization of devices is pervasive in the electronics, medical and the energy industries and there is a great demand for these devices to have very high form and surface finish. At the nanoscale, machining phenomena take place in a small limited region of tool – workpiece interface, which often contains a few atoms or layers of atoms. Currently, it is very difficult to observe the diverse microscopic physical phenomena occurring at that length scale through experiments and dimension problems limit the use of analytical and empirical models [1]. The interface at this nanometre level may not be considered as a continuous media or homogeneous as assumed by continuum mechanics, so the analysis should be based on discrete atoms whose interactions are governed by appropriate interatomic potentials. The use of Molecular Dynamics (MD) simulation has proved to be an effective tool for the investigation of machining processes at the nanometre scale. The method gives higher resolution of the cutting process than what is possible by continuum mechanics on that length scale.

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 simulation method has extended from Physics to Materials Science and now to Mechanical Engineering. Rentsch and Inasaki [3] modelled a copper workpiece and a diamond tool using the Lennard-Jones potential for the copper atom interactions. They observed a build-up phenomenon after 25000 time steps, while keeping the tool rigid. Komanduri et al [4] used copper workpiece and an infinitely hard tungsten tool for their simulation. They used Morse potentials and a cutting speed of 500m/s.
Many existing MD simulation studies on nanometric cutting have been limited to single pass tool or simple line-type groove. As an extension of the single pass studies, Zhang et al [5] modelled folder-line grooves for AFM-based nanometric cutting process of copper with diamond tool. They used the EAM potential for the copper-copper interactions and the Morse potential for the copper-diamond interactions. They treated the diamond tool as rigid and concluded that the normal, lateral and the resultant forces were almost symmetric with respect to the critical folder angle of 45°. Shi et al [6]

investigated the multi-groove simulation of single-point tuning of copper with diamond tool. They used a two-groove cutting procedure and modelled the copper-copper and the copper-diamond interactions by using the Morse potential. They also treated the tool as a rigid body and observed that the tool forces increase with increase in feed rate and depth of cut. In practice, most machining processes involve the use of multiple passes to create new surface patterns and the diamond tool is deformable. To address this problem, a multi-pass cutting was employed in this study to simulate the surface creation in single point diamond turning.

The MD Simulation Methodology

The configuration has a total of 54232 atoms. The workpiece consists of 43240 copper atoms with the FCC lattice. It includes 3 kinds of atoms namely; boundary atoms, thermostat atoms and Newtonian atoms (See Fig. 1). The cutting tool consists of 10992 carbon atoms with diamond lattice structure. Fig. 2 shows a diagram of the machined grooves with passes 1, 2 and 3.

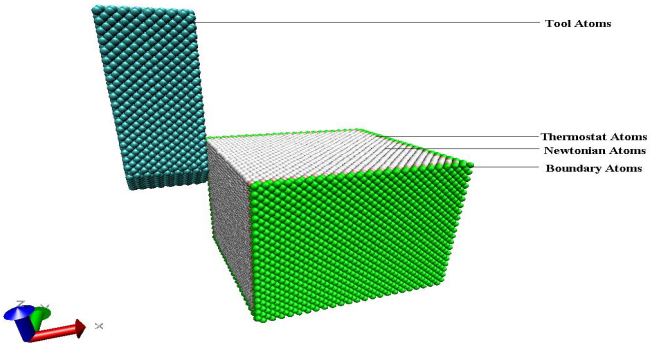


Figure 1: The MD Simulation Model

The simulation conditions applied in this study are the following, viz; Bulk temperature is 293K, the cutting direction is along the x-axis, the cutting speed is 150m/s, the cutting depth is 1.5nm, feed is 1.5nm, the time step is 0.3fs and the simulation run is 150000 steps.

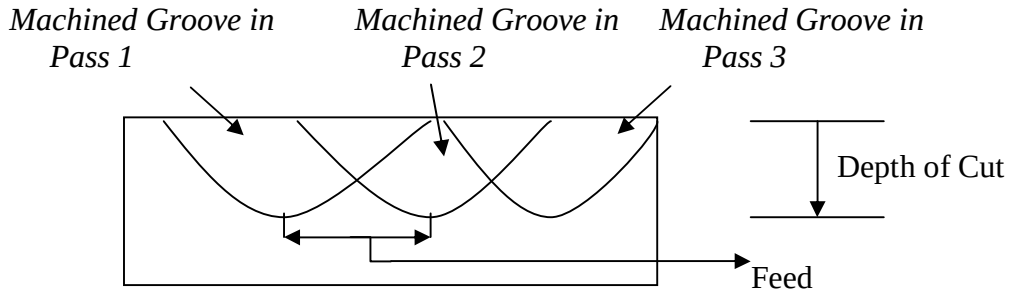


Figure 2: Cross Section of the Machined Grooves with Passes 1-3 (direction of cut is perpendicular to the paper face)

The cutting tool is fairly pointed shaped. The boundary atoms are kept fixed to reduce edge effects. The thermostat atoms conduct the heat generated during the cutting process out of the cutting region. This is achieved by the velocity scaling of the thermostat atoms, (with the conversion between the kinetic energy (KE) and temperature via Eq. 1 [7, 8]);

$$\sum_i \frac{1}{2} m_i v_i^2 = \frac{3}{2} N k_B T_i . \qquad (1)$$

Where m_i is the mass of the ith atom, v_i is the resultant velocity of the ith atom, N is the number of the thermostat atoms, T_i is the temperature of the ith atom and k_B is the Boltzmann constant ($1.3806504 \times 10^{-23}$ JK^{-1})

Whenever the temperature of the thermostat atoms exceeds the preset bulk temperature of 293K, their velocities are scaled by using Eq. 2 [9, 10];

$$v_{i,new} = v_i \sqrt{\frac{T_{desired}}{T_{current}}} \,. \tag{2}$$

Where $T_{current}$ is the current temperature that is calculated from the KE and the $T_{desired}$ is the desired temperature. The Newtonian atoms obey the Newton's equation of motion. The LAMMPS MD software [11] was used for the simulations and the VMD software [12] was used for the visualization of the results.

The modelling parameters for potentials

Many researchers sometimes use different interatomic potentials for nanometric machining simulation without justifications. In previous studies, it has been established that the EAM potential is very suitable for the Cu-Cu interactions [13, 14] and for the Cu-C interactions, the Morse potential is a good choice [15].

Embedded-Atom Method Potential (EAM) (Eq. 3) [16] (*For the Cu-Cu interactions)*

$$E_{tot} = \sum_i G_i(\rho_{h,i}) + \frac{1}{2}\sum_{i,j} V_{ij}(r_{ij}) \,. \tag{3}$$

Where $\rho_{h,i}$ is the total electron density at atom i due to the rest of the atoms in the system.
G_i is the embedding energy for placing an atom into the electron density, $V_{i,j}$ is the short range pair interaction representing the core-core repulsion, r_{ij} is the separation of atoms i and j

Morse Potential (Eq. 4) [17] (*For the Cu-C interactions)*

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

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
The parameters used in the simulations are below, [18];

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

The cut-off distance chosen was 6.4 Angstroms (that is, the interactions between atoms separated by more than this distance are neglected).

Tersoff Potential (Eq. 5) [19] *(For the C-C interactions)*

$$E = \sum_i E_i = \frac{1}{2}\sum_i \sum_{i \neq j} V_{ij} \,. \tag{5}$$

and,

$$V_{ij} = f_C(r_{ij})[a_{ij} f_R(r_{ij}) + b_{ij} f_A(r_{ij})]$$

where

$$f_R(r) = A\exp(-\lambda_1 r),\ f_A(r) = -B\exp(-\lambda_2 r),\ a_{ij} = (1+\alpha^n \eta_{ij}^n)^{-1/2n},\ b_{ij} = (1+\beta^n \zeta_{ij}^n)^{-1/2n}$$

$$f_C(r) = \begin{cases} 1, & r < R-D \\ \frac{1}{2} - \frac{1}{2}\sin\left[\frac{\pi}{2}(r-R)/D\right], & R-D < r < R+D \\ 0, & r > R+D \end{cases},\quad \eta_{ij} \sum_{k(\neq i,j)} f_C(r_{ik}) \exp\left[\lambda_3^3 (r_{ij} - r_{ik})^3\right]$$

$$\zeta_{ij} = \sum_{k(\neq i,j)} f_C(r_{ik}) g(\theta_{ijk}) \exp\left[\lambda_3^3 (r_{ij} - r_{ik})^3\right],\ g(\theta) = 1 + \frac{p^2}{q^2} - \frac{p^2}{\left[q^2 + (h - \cos\theta)^2\right]}$$

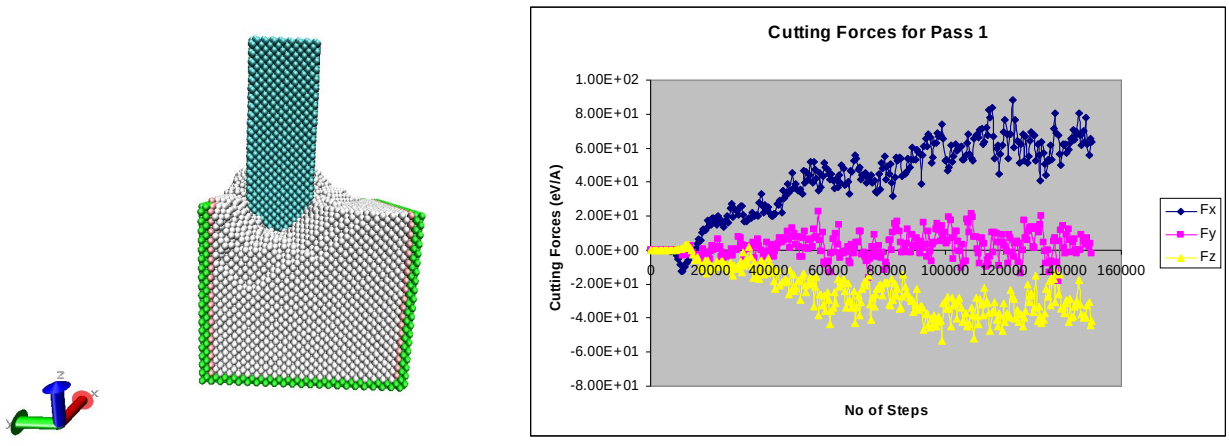
Where R and D are cutoff parameters; $A, B, \lambda_1, \lambda_2, \lambda_3, \alpha, \beta, n, p, q, h$ are fitting parameters of the Tersoff potential.

The simulation parameters used for carbon, are given as [19, 20, 21];

A(eV) $= 1.3936 \times 10^3$; B(eV) $= 3.467 \times 10^2$; $\lambda_1 (nm^{-1}) = 34.879$; $\lambda_2 (nm^{-1}) = 22.119$; $\alpha = 0.0$;

$\beta = 1.5724 \times 10^{-7}$; n $= 7.2751 \times 10^{-1}$; p $= 3.8049 \times 10^4$; q = 4.384; h = -5.7058×10^{-1};

$\lambda_3 (nm^{-1}) = 22.119$; R (nm) = 0.18; D(nm) = 0.02.



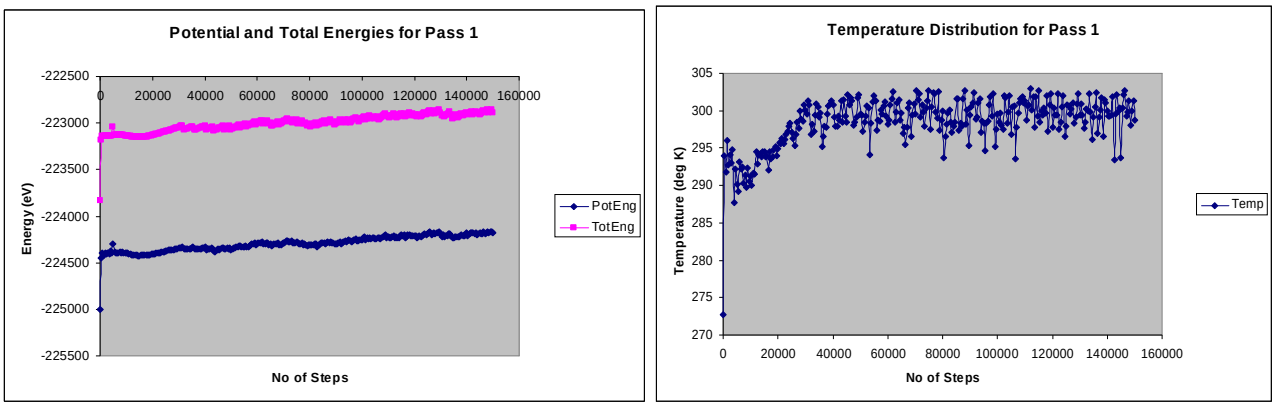
(a) (b)

Figure 3a: Simulation of Pass 1 Cutting; 3b: Cutting Forces for Pass 1

Simulation Results and Discussion

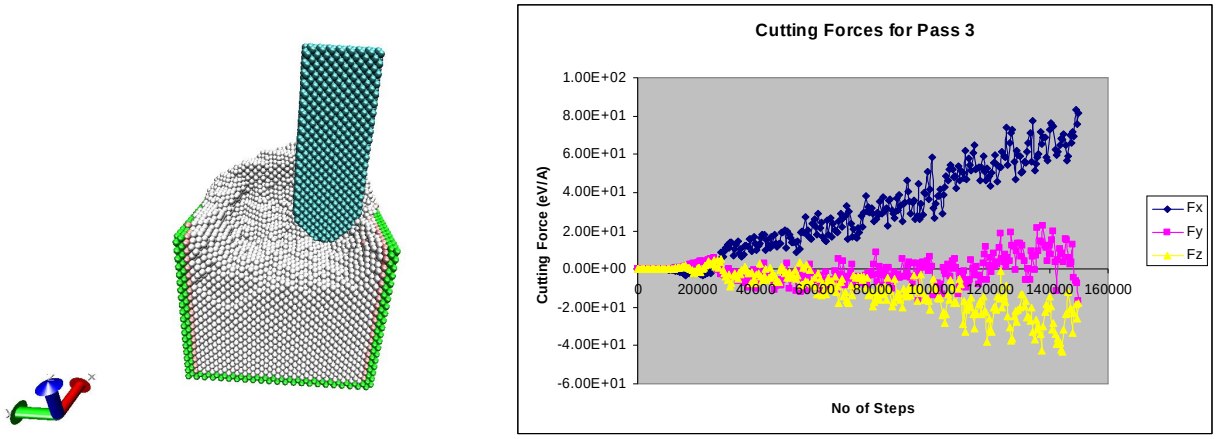
Figs. 3a, 3b, 4a and 4b show the simulation results for the pass 1 groove cutting. Figs 5a, 5b, 6a and 6b show the results for the pass 3 groove cutting. F_x, F_y and F_z are the tangential, lateral and normal components of the cutting forces respectively. The average F_x decreases with the consecutive passes in the simulation, i.e. from 41.5063 eV/A in pass 1, to 30.98684 eV/A in pass 2, and then to 29.57385 eV/A, in pass 3. (1eV/A = 1.602nN). The average F_z also decreases in a similar way. This is so because there are less material to be removed during the passes 2 and 3 compared to pass 1. F_y should be zero theoretically, but it varies around zero for the pass 1 simulation. This shows the atomic vibration effects during the cutting process. However, for passes 2 and 3, F_y is biased towards the positive side because the cutting cross section is asymmetry and skewed to the right. The cutting forces, the potential energy, the total energy, and the temperature distribution are comparable for passes 2 and 3, so only that of pass 3 are shown. The temperature sharply increases initially for pass 1 and stabilizes as the time step increases. For passes 2 and 3, the temperature

distribution is fairly stable as the time step increases. This is because at the start of the pass 1 cut, the interface between the tool edge and the workpiece generates an initial high temperature, which is later conducted away and stabilizes. For pass 2 and 3, there is less material to be removed, so there is no much initial temperature built-up. Also, for passes 2 and 3, the potential and the total energies decrease initially and then stabilize. This may be because the tool initially engaged the asymmetrical atomic structure left after the previous pass.



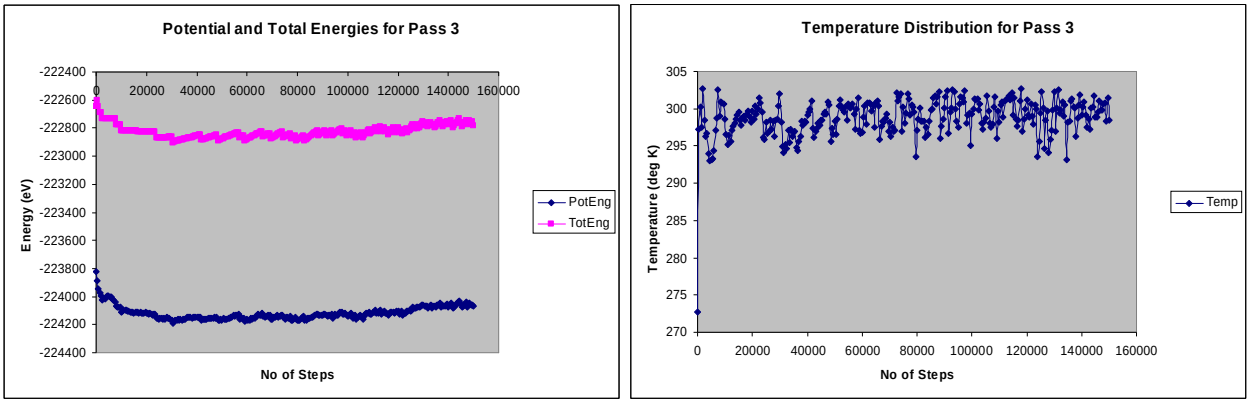
(a) (b)

Figure 4a: Potential and Total Energies for Pass 1; 4b: Temperature Distribution for Pass 1



(a) (b)

Figure 5a: Simulation of Pass 3 Cutting; 5b: Cutting Forces for Pass 3



(a) (b)

Figure 6a: Potential and Total Energies for Pass 3; 6b: Temperature Distribution for Pass 3

Summary

The MD simulation of multi-pass nanometric machining procedure has been clearly demonstrated. It was observed that the average tangential and the normal components of the cutting forces decrease with the consecutive passes. The ratio of the tangential to the normal force component is in the range 1.77 to 2.69 for the three passes. Also, the lateral force components are affected by the atomic vibrations and the cutting cross sectional area.

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