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Nano-Grooving on Copper by Nano-Milling and Nano-Cutting

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Abstract. This paper uses the molecular dynamics simulation to investigate the quality of nano-scale grooving on mono-crystalline copper by high-speed nano-milling and nano-cutting. The results reveal that nano-milling produces a high-quality nano-groove with smooth surfaces in comparison with a nano-cutting. It is also interesting to note that the machined workpiece subsurface can be free from dislocations.

Introduction

Miniaturized components with nano-scale surface features have wide applications in the fields of aerospace, automotive, electronics, environment, renewable energy and telecommunications [1 - 4]. To generate complex surface profiles on materials, a mechanical nano-machining process is often more superior than ion implantation- and lithography-based machining, because the former is usually more efficient, portable and cost-effective, and consumes less energy.

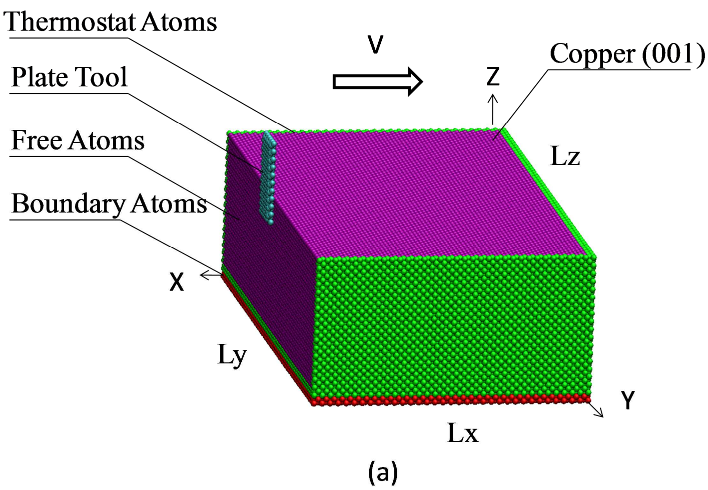
To understand the fundamental material removal mechanisms associated with the mechanical nano-machining processes, substantial research has been conducted on nano-indentation, nano-grinding, nano-cutting and nano-polishing. For example, Zhang and Tanaka [5] investigated the deformation mechanisms of copper under the contact sliding of a diamond tip. They found that material removal can take place only when the depth of the cut reaches a critical value below which no-wear, adhesion, or ploughing deformation will happen. In studying the three-dimensional nano-cutting of copper [6], Tanaka and Zhang found that complex dislocations in the machined workpieces are the main mechanism of subsurface damage. Ye, et al. [7] simulated the nano-cutting of copper with the embedded atom method, and observed that at a high cutting speed a machined surface would be rough but without dislocations; while at a low cutting speed the surface could become smooth, but dislocations were generated. To date, however, little has been done on the understanding of nano-milling, although it could be an effective process for making complex three-dimensional surfaces [4].

This paper will investigate the mechanics and material removal mechanisms associated with the nano-milling of nano-grooves on mono-crystalline copper. Three dimensional molecular dynamics (MD) simulation will be carried out to analyze the deformation of the material. Nano-cutting will also be studied for comparison.

The MD Simulation

It was found that a control volume of 12.3 nm × 21.7 nm × 6.5 nm consisting of 154,457 atoms is sufficient to avoid the boundary effect in the MD simulation of nano-milling and nano-cutting. To eliminate the rigid body motion, two layers of atoms at the bottom of the control volume were fixed to the space – called boundary layers for convenience. On the other hand, to have reasonable heat conduction outwards the control volume, two layers of thermostat atoms were arranged around the control volume, except the front and top surfaces, as shown in Fig. 1(a). The nano-milling and nano-cutting were carried out along the $[\bar{1}00]$ direction on the (001) surface under similar machining conditions. The nano-milling/cutting tool was a rigid diamond plate of dimensions 0.1 nm × 1.8 nm × 3.6 nm, as shown in Fig.1 (b). In nano-cutting, the tool moved with speed V as indicated in Fig. 1(a);

but in nano-milling, the tool rotated about z-axis at an angular velocity ω while moving at the speed V, where the z-axis is the symmetrical axis of tool width. In both the nano-milling and nano-cutting processes, the tool was initially positioned 0.3 nm away from the left edge of the control volume. The depth of cut was 0.9 nm.



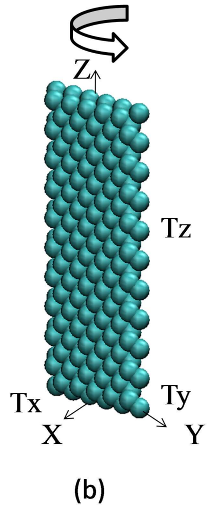


Fig. 1. The molecular dynamics model for the nano-milling and nano-cutting. (a) the control volume of the mono-crystalline copper workpiece showing the initial position of the cutting/milling tool, where green atoms are thermostat atoms, red atoms are fixed boundary layers and purple atoms are Newtonian atoms, (b) the nano-milling/cutting tool.

The simulation parameters used in this study are summarized in Table 1. In order to stabilize the average temperature at 293 K, heat generated during the machining process was conducted away through the thermostat atoms by (i) scaling for rapid thermal energy conduction, and (ii) scaling velocities of thermostat atoms at each step [8]. During the nano-milling process, chips are removed every one fifth of the rotational cycle in order to get a clear visualization of a machined surface.

Table 1. MD simulation parameters

Materials	Workpiece: Copper (FCC)	Tool: Diamond (rigid)
Dimensions [nm^3]	12.3× 21.7 × 6.5	0.1× 1.8× 3.6
Time step [fs]	10	
Cutting depth [nm]	0.9	
Angular speed ω [rpm]	5.2×10^{10}	
Feed rate [m/s]	90.2	

Table 2. Morse potential parameters

	Cu-Cu	Cu-C
D_e [ev]	0.342	0.087
α [nm^{-1}]	13.59	51.40
r_e [nm]	0.287	0.205

The Cu-Cu interactions and Cu–C interactions were described by the Morse potential [5] given by

$$V(r_{ij}) - D_e = D_e\left(e^{2\alpha(r_e - r_{ij})} - 2e^{\alpha(r_e - r_{ij})}\right) \quad (1)$$

where r_e is the equilibrium distance between atoms i and j, r_{ij} is the instantaneous distance between atoms i and j, D_e is the cohesive energy between the two atoms and α is the parameter obtained from the Debye temperature [5]. The parameters for the Cu-Cu and Cu-C interactions are listed in Table 2. This potential has been used extensively.

Results and discussion

Heat conduction. A high speed machining process can generate a large amount of heat. In metals the thermal energy is mainly conducted by electron movements. However, an MD simulation accounts for the thermal energy caused by the movement of atoms and the temperature control is by scaling the velocities of atoms. Thus an MD simulation cannot capture the thermal transport by electron movements. To compensate this, the gradient in thermal field should be scaled so as to coincide with that obtained by continuum conduction theory, as pointed out by Shimada et al [9]. In this work, the velocity of the atoms were scaled by

$$U_i = \left\{1 - \beta_1\left(1 - \frac{V_m}{|V_i|}\right)\right\}V_i \tag{2}$$

where U_i is the scaled velocity of atom i, β_1 is a material constant for copper, V_m is the mean square velocity and V_i is the velocity of atom i before scaling. Then the velocities of atoms are rescaled to keep the total energy unchanged [5, 8]. In this way, a reasonable result for thermal field can be achieved in the MD simulation of a metal machining process.

Nano-milling. In the nano-milling process the three components of the forces, F_x, F_y and F_z, represent the feed force, cross feed force, and the normal force, respectively. Fig. 2 shows the variations of these force components with the milling distance. At the early stage of the process, i.e., as the milling tool approaches the workpiece, the interactions between the tool and workpiece atoms are rather small. With the tool edge advancement, the tool-workpiece atomic interactions become periodic because the tool rotates during its feeding operation. As a result, the force components fluctuate correspondingly. The cross feed force F_y is much higher than the other components F_x and F_z. This is because in the milling (see the conditions in Table 1), the rotation is much larger compared with the feed rate in the X-direction.

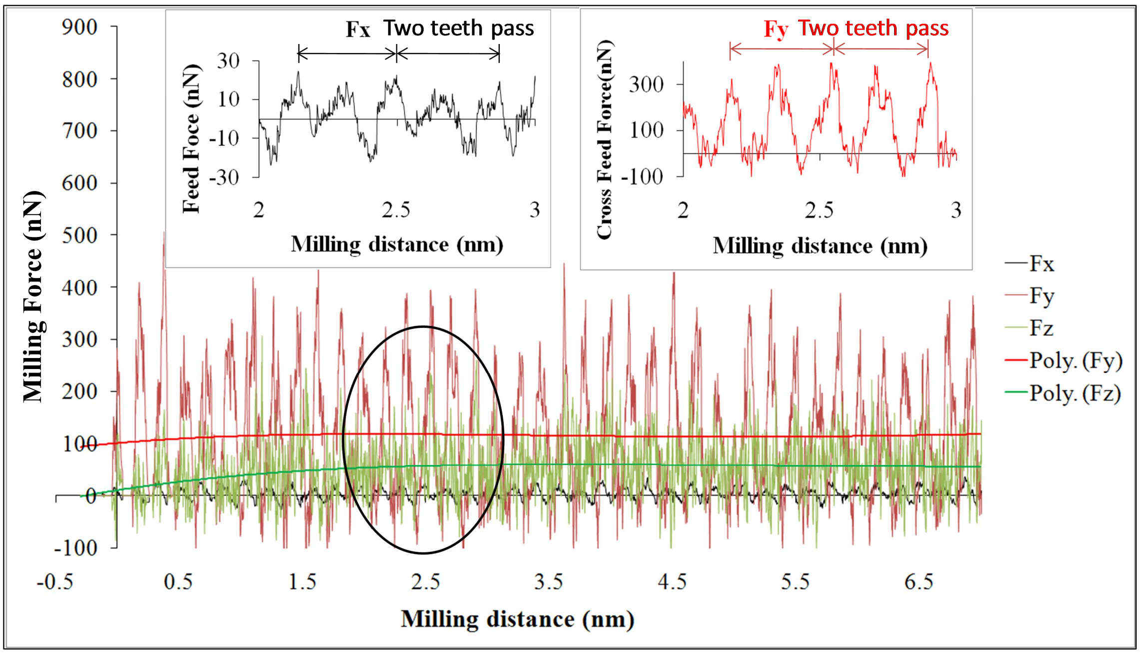


Fig. 2. Variation of the milling force (The top insertions are the enlargements of the circled region)

For a better visualization of the force variations, enlargements of the region circled are inserted at the top of Fig. 2. The time between homologous points on every other peak corresponds to the teeth passing period which has been calculated based on the rotational speed of the tool. The average values of the cross feed force and normal force are 102 nN and 47.8 nN, respectively.

Nano-cutting. In this case, the three components of the forces, F_x , F_y and F_z, represent the feed force, lateral force and normal force, respectively.

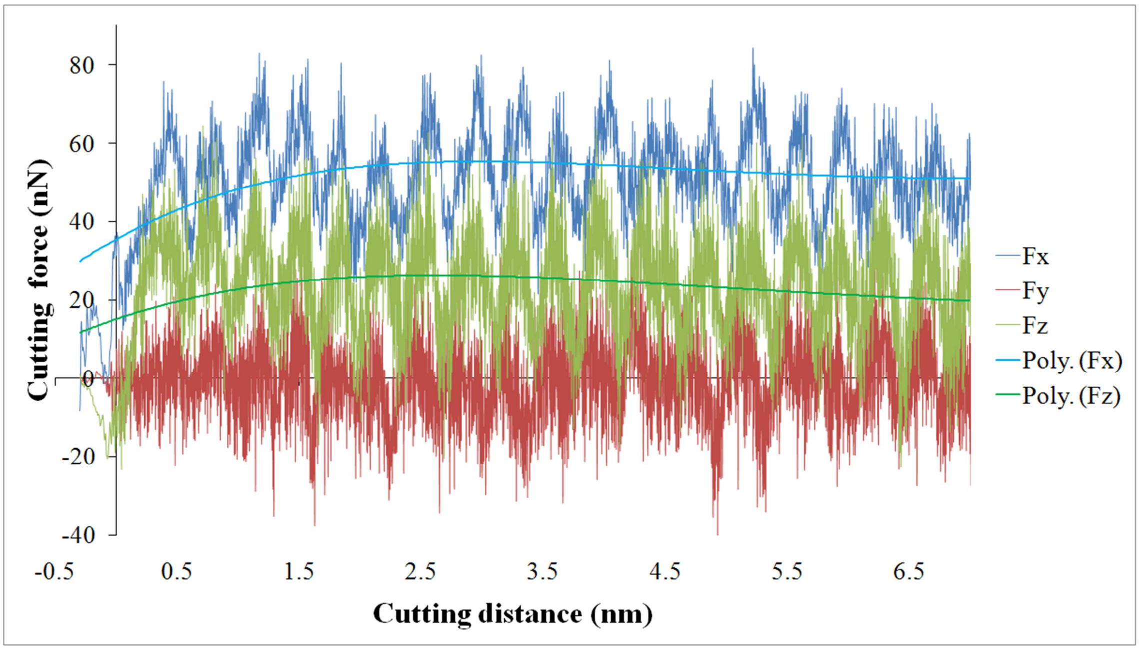
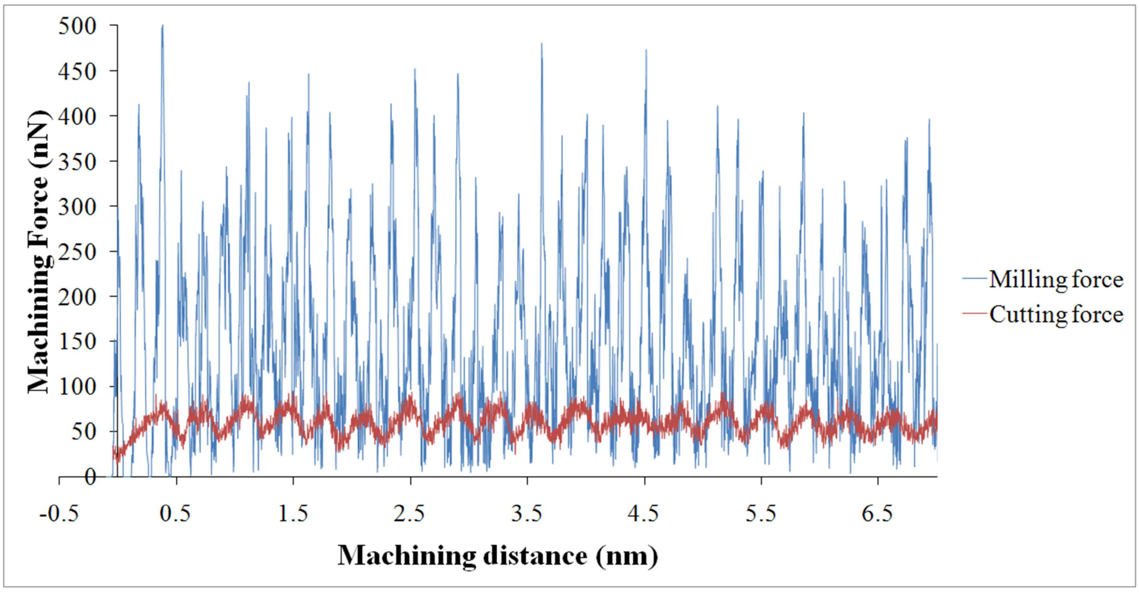


Fig. 3. Variation of the cutting forces.

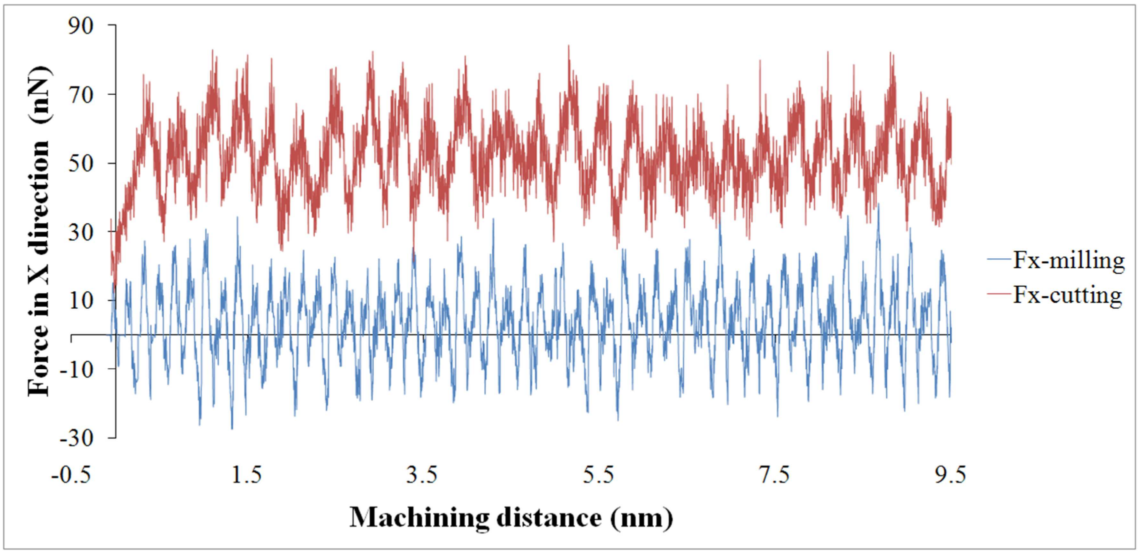
Fig. 3 shows that all three force components vary around zero when the tool approaches the workpiece, but rise sharply once the tool penetrates into the workpiece. During the cutting, the force components fluctuate with the cutting distance, but the fluctuation is smaller than that in milling. Such kind of fluctuation is expected because the force reflects the discontinuous interactions between the tool and workpiece atoms. The average values of F_x, F_y and F_z are 55nN, 8nN and 25nN, respectively. Obviously, the lateral force is very small because the cutting tool is symmetrical about the cutting axis.

Fig. 4 compares the total force, feed force and the normal force of nano-milling with those of nano-cutting. From Fig. 4(a), it can be seen that the total force in nano-milling is larger than that in nano-cutting and the cross-feed force derived from the very high rotation motion in nano-milling is responsible for this. Fig. 4(b) shows that the feed force in cutting is larger than that in milling. This is because in milling, the tool rotates, and only the cutting edge of the tool is in contact with the workpiece. In cutting, however, the full width of the tool is in contact with the workpiece. Hence the contact area between the cutting tool and workpiece is much greater compared to the scenario of nano-milling, leading to a relatively larger feed force. The difference between the normal forces of nano-milling and nano-cutting is cause by their different cutting edge trajectories.

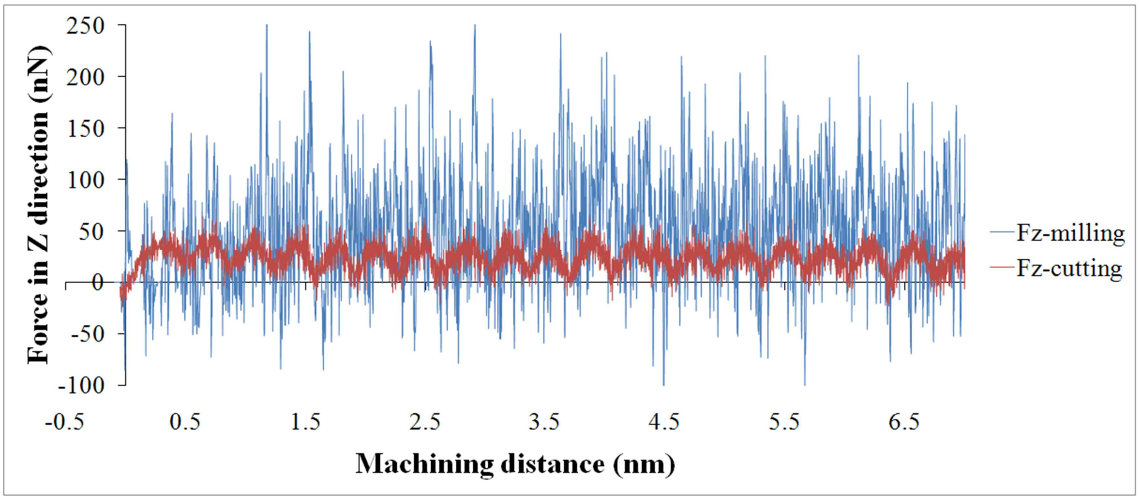
Fig. 5 compares the grooves produced by nano-milling and nano-cutting. It can be seen that the groove from the former has a more defined shape and is smoother. However, at the depth of cut studied here, the subsurface of the workpiece by either nano-milling or nano-cutting is free from dislocations.



(a)

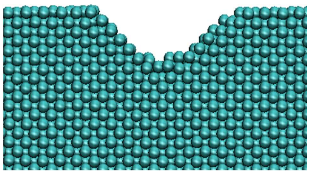


(b)

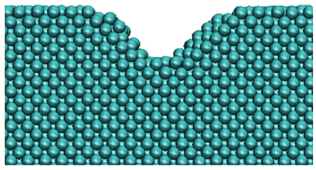


(c)

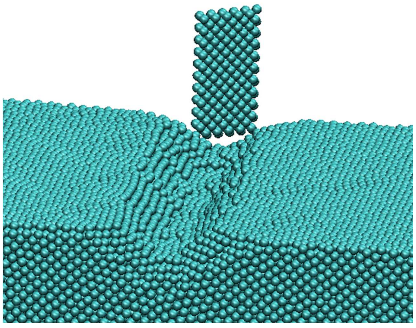
Fig. 4. Comparison of nano-machining forces. (a) total force, (b) feed force, and (c) normal force



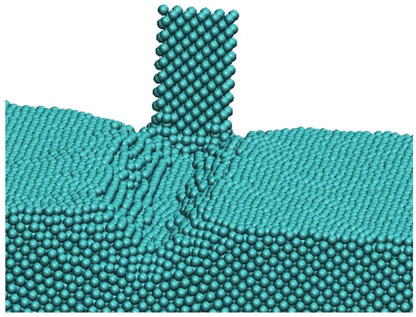
(a) Front view of the groove by nano-milling



(b) Front view of the groove by nano-cutting



(c) A portion of the groove after nano-milling



(d) A portion of the groove after nano-cutting

Fig. 5. Groove quality by nano-milling and nano-cutting

Conclusion

Based on the analysis and discussion given above, the following conclusions can be made:

(1) The nano-groove made by nano-milling has a better profile and smoother surface.
(2) When using a plate tool, a larger force is required for nano-milling compared to nano-cutting, due to the greater cross-feed force in the former.
(3) The machined surfaces are free from dislocations.

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