Simulation and optimization of surface roughness and cutting force in dynamic ploughing process of single crystal copper using molecular dynamics method

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ABSTRACT

Surface roughness is one of the most important characteristics in nanomachining products. In this paper, using molecular dynamics simulation in LAMMPS software, the process of dynamic nano ploughing of single-crystal copper workpiece is investigated by a diamond tool, and the quality of the production surface and cutting forces were investigated as two target parameters. The effect of parameters of dynamic nano- ploughing process such as depth of cut (DOC), amplitude (R) and frequency (ω) of cutting tool vibration on cutting force and surface roughness has been investigated by calculating average roughness (R_a). Also, in order to more closely examine the effect of parameters and their interaction on each other, Taguchi method has been used to design experiments. The simulation results show that the characteristics of cutting depth, amplitude and frequency of cutting tool vibration have the greatest effect on surface smoothness and cutting forces, respectively. Based on the presented results, it has been determined that the surface roughness can be improved in different machining conditions based on the selection of parameters, and it is necessary to check their conditions together well before selecting these parameters. Also, finally, by using Taguchi method, the optimal values of dynamic ploughing parameters were obtained to achieve the best surface smoothness and the lowest cutting force in certain dimensions as described by DOC=2.5 Å, R=0.1 Å and ω=50 KHz.

KEYWORDS

Dynamic ploughing, Molecular dynamic method, Surface roughness, Taguchi method, Single crystal copper.

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1. Introduction

Copper nanomachining has wide applications in the field of laser optics, linear accelerator cavity, and semiconductor technology. In addition, single crystal copper also acts as a substrate material for the growth of graphene, which has exceptional electronic properties. Since nanomachining involves the interaction of atomic groups and the behavior of materials has a discrete nature, continuum mechanics analysis does not work well for it. Therefore, molecular dynamics simulation becomes an essential tool in investigating the nanoscale cutting process [1]. In the nanomachining process, the shear forces are the interparticle forces that are the result of the interaction between the tool and the workpiece particles [2]. Due to the high requirements of ultra-precise machine tools, testing methods and machining conditions, it is very difficult to investigate the mechanism of nanomachining using experimental methods [3]. The best way to gain a proper insight into these processes is to use atomic simulation methods for modeling at the nanometer scale. Molecular dynamics is a comprehensive physical model that includes intrinsic information such as geometry, velocity and forces that are effective in atomic behavior at this scale [4].

Dynamic plowing refers to the use of tool tip vibration to scratch the surface and machining nanostructures [5]. Based on the literature review, it was determined that the effect of the machining parameters such as depth of cut and the amplitude and frequency of the cutting tool vibration on reducing the cutting forces and surface roughness in the dynamic nano ploughing of single-crystal copper workpiece has not been studied. Therefore, in this research, the effect of these parameter on the surface roughness of the workpiece are simultaneously investigated. Also, using Taguchi's optimization method and test design, initial optimal parameters are obtained in order to achieve the maximum signal to noise ratio.

2. Methodology

In this research, the three-dimensional simulation of the nano machining process was performed using Lamps molecular dynamics software, and the outputs were analyzed using Ovito software. In the molecular dynamics model developed in this article, the workpiece is made of single crystal copper and the tool is made of diamond. According to Figure 1, in order to match the results with reality, three Newtonian layer, boundary layer and thermostat layer have been considered for tools and workpieces. The size of the workpiece is considered $\left[400\text{Å}\times165\text{Å}\times70\text{Å}\right]$ where contains 412425 atoms.

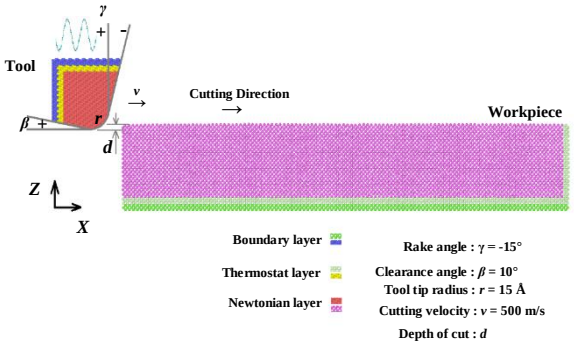

Figure 1. Specifications of the molecular dynamics model

In this research, the geometrical characteristics of the cutting tool and the nano machining process are selected from reference [6]. Further, considering the requirement to express interatomic forces based on experimental potentials in molecular dynamics, for the three atomic interactions copper-copper, carbon-carbon and carbon-copper, respectively, the potential functions of the embedded atom method [7], Tersoff [8] and Morse [9] were used. Also, the initial temperature of the system is considered to be 300^0 k. Then, with the passage of time, the model reaches stability and dynamic equilibrium based on the initial conditions of temperature, force, boundary, potential and dimensions. Finally, the cutting tool starts cutting at a constant speed of 500 m/s in the direction of the longitudinal axis X and oscillates according to the vibration function $Rsin(\omega t)$, and the simulation is completed.

In molecular dynamics simulations, in order to prepare the thermodynamic conditions of the model at the beginning of the simulation and during the process, the concept of thermodynamic ensembles is used. In this research, in order to balance the model as much as possible before the cutting process, the system was placed in the state of minimum total energy, and then, in order to balance and remove the residual stresses, the NPT ensemble was used. Also, for the simulation of the thermostat layer, in order to keep the temperature constant, the NVT ensemble, and for the Newtonian layer, for the purpose of cutting, the NVE ensemble has been used.

The target parameters in this research are surface roughness and chipping force. In order to analyze the surface roughness, the average roughness characteristic was used.

3. Discussion and Results

In this section, using the Taguchi method, three parameters in three levels (according to Table 1) are investigated and the effects of changing these input

parameters on the surface roughness and cutting force outputs are studied. For this purpose, in the first stage, the optimal values of the input parameters are obtained with the minimum test and with 9 runs with different specifications, and then, in order to analyze the interaction of the input parameters, with the maximum test and with 27 runs, in addition to the optimal values, the interaction of the input parameters is also examined.

Table 1. Levels of input parameters

	Input parameters		
	R (Å)	*ω* (KHz)	*DOC* (Å)
Levels	0.1	10	2.5
	0.2	20	5
	0.5	50	10

According to the simulation results, for the fixed depth of cut and tool oscillation amplitude, the cutting force is reduced at higher tool oscillation frequencies. This is due to the increase in the kinetic energy of the tool at higher frequencies, which increases the kinetic energy of the workpiece particles at the moment of contact and causes easier separation of the particles from the workpiece. Also, increasing the depth of cut and the tool oscillation amplitude has also increased the cutting force. In both cases, with the increase of the relevant parameter, the number of atom bonds of the work piece that must be broken in order for the cutting process to take place increases, which has increased the cutting force.

The optimal values of dynamic ploughing parameters are obtained to achieve the best surface smoothness and the lowest cutting force as described by DOC=2.5 Å, R=0.1 Å and ω=50 KHz. The simulation results for a sample with unfavorable surface smoothness and optimized sample are presented in Figures 2 and 3.

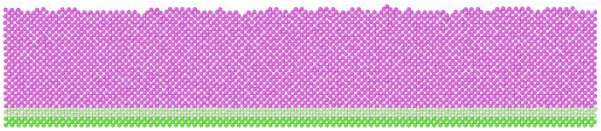

Figure 2. Nano ploughing surface using input parameters DOC=2.5 Å , ω=50 KHz, R=0.2 Å

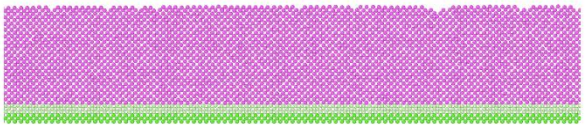

Figure 3. Nano ploughing surface using input parameters DOC=2.5 Å , ω=50 KHz, R=0.1 Å

4. Conclusions

In this paper, molecular dynamics simulation has been used to investigate the effect of depth of cut (DOC), amplitude (R) and frequency (ω) of the tool oscillation on the dynamic nano ploughing process of a diamond tool on single crystal copper workpiece.

In order to determine the optimal input conditions to achieve the best surface smoothness and the lowest cutting force, the Taguchi method has been used. Using this method, by designing the experiments and with the least number of runs, the optimal parameters were predicted with proper accuracy, and in addition, the effect of these parameters on the output was investigated. The simulation results shown that by using these optimal input parameters, the average surface roughness R_a=0.91 Å and the chip removal force F=22.4 nN can be achieved.

5. References

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