Nanometric face milling simulations using MD method

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Abstract. Face milling is considered as one of the most important methods in order to produce parts with high quality surfaces and considerable dimensional accuracy in a relatively short time. Investigation of the effect of process parameters on the outcome of this process is usually conducted experimentally or computationally by soft computing or numerical methods. However, when it is desired to study face milling in the nanoscale, experimental cost can be extremely high and numerical methods such as the Finite Element Method is unable to be employed, as it is a method mainly suited for continuum mechanics. Thus, a method such as Molecular Dynamics can be used to perform simulations of face milling in the nanoscale. In this work, cases with cutting tools with one and three cutters, moving at different feed values are considered and results concerning chip morphology and cutting forces are presented.

1. Introduction

Milling is essential in manufacturing industry in order to fabricate efficiently a wide variety of parts, with different levels of geometric complexity and dimensional tolerances. The rapid progress of manufacturing and the requirements of high-end industries such as the electronics industry lead to an increasing interest in micro and even nano-manufacturing processes. The capabilities of nano-milling to act as a viable alternative of established nano-fabrication techniques, such as lithography or nano-printing are considered as promising [1-3].

For the establishment of nano-milling, it is necessary to determine its characteristics in respect to the process parameters, as well as the underlying physical phenomena occurring during material removal. Afterwards, it will be able to determine the optimum process parameters, with a view to reduce machining time and prevent excessive subsurface damage to the workpieces. These investigations should be carried out experimentally, but due to the relatively high cost of performing experiments in the nanoscale or even the inability to accurately measure physical quantities during these experiments, theoretical investigations using proper computational techniques should be also performed. As the Finite Element Method (FEM) is not able to simulate explicitly the phenomena occurring in the nanoscale, the Molecular Dynamics method is adopted for nanoscale simulations. Nano-machining simulations conducted with the aid of MD method have been reported since the early 1990s. One of the earliest works, was that of Rentsch and Inasaki [4] who studied nano-grinding with a 3D model of a diamond abrasive grain and a copper substrate. This model was created to investigate material removal mechanisms in the nanoscale. In another work [5], they studied the phenomenon of

crack initiation during nano-grinding, as well as the integrity of machined surface. In a pioneering study, Komanduri et al. [6] employed MD models with large negative rake angle tools in order to simulate nanometric grinding and were able to detect dislocations in the workpiece, determine the subsurface deformation and determine the variation of cutting forces and energy in several cases. Apart from nano-grinding, models for general machining [7] and various models of polishing [8] have been presented in the relevant literature. Nevertheless, models related to nano-milling have not been thoroughly investigated yet.

Cui et al. [9] created an MD nano-milling model in order to investigate the quality of produced grooves. In this study, a cutting tool with two cutting edges moving at a realistic way and a copper substrate were employed and the different characteristics of nano-milling in comparison to nano-cutting were determined. In another study [1], they compared the cases of end-milling and peripheral milling in nanometric level using suitable MD models. When comparing the outcome of these two processes, it was found that cutting forces were lower in end-milling and that this process was more stable; however with peripheral milling, grooves of better quality were able to be obtained. The effects of various process parameters such as depth of cut, feed rate, angular speed and shape of cutting tool on cutting force and groove quality were investigated by Cui et al. [10]. It was found that the cutting tool with four cutting edges was performing milling with less fluctuations of the cutting force and that increase of feed and depth of cut led to higher cutting forces. Furthermore, it was shown that the depth of cut was the most important parameter, which affected the quality of produced grooves.

More recently, another comprehensive work regarding nano-milling in order to study the material removal mechanisms was conducted by the same scientific group [11], in which they assessed the groove quality which was obtained. For that purpose, simulation with cutting tools with different dimensions, different feed rate and rotational speed values were performed. It was found that the most important factors affecting the groove profile are the cutting speed and groove dimension factors and that profile quality increases by decreasing the former and increasing the latter. Similar results are also summarized in the work of Cui and Zhang [12]. Besides these models, some researchers have proposed different nano-milling models as well. Olufayo et al. [13] used a box-shaped cutting tool in order to study milling on copper workpieces. Furthermore, Wu et al. [14] investigated the characteristic of nano-milling by conducting simulations with a rotating conical cutting tool. However, these models describe mainly the formation of nano-grooves by nanometric milling cutting tools, but no study on face milling with a cutting tool with multiple cutting inserts is yet presented.

In the present work, an MD model for nanometric face milling is introduced, with a view to explore the possibilities of this type of milling and study various characteristics of the process. For that reason, simulations using cutting tools with 1 and 3 cutters, at various feed rates will be performed on copper substrates. By analyzing the results regarding chip morphology and cutting forces, useful observations on the underlying phenomena of nanometric face milling are conducted.

2. Molecular Dynamics method

As it was aforementioned, due to the fact that it can more realistically and accurately simulate machining in the nanoscale, where matter is not a continuum, MD method is preferred for these simulations. Hereafter, a brief description of the method is attempted, with a view to present the basic characteristics of this method. Using MD method, the system comprising the cutting tool and the workpiece is represented by its atomistic structure. The atoms of the cutting tool and the workpiece can move freely under the influence of interatomic forces, they can be fixed in a specific position, or move with a constant speed as a rigid body. For atoms which can move freely, the forces exerted on them are summed and they move according to the second law of Newton. Interatomic forces are calculated with the aid of appropriate potential functions, such as Morse function or Embedded Atom Model (EAM) function which is suitable for metals. The atomic trajectories are calculated by integrating the Newtonian equation of motion and after the simulation is completed, atomistic forces, temperatures, stresses and subsurface damage can be determined. Although modern MD software can

provide relatively lower computational cost, it is still difficult to perform simulations on systems exceeding 10^6 atoms in most cases and thus, simulations are limited to nm size substrates.

3. Methodology

In the present work, various cases of nano-milling of single-crystal copper (FCC) substrates with two different cutting tools and at three different feed rate values are studied by means of MD method. The depth of cut in all cases is the same, namely 0.6 nm, the rotational speed of the cutting tool is 50.24 rad/ps, the feed rate values are 100, 200 and 300 m/s and the total cutting length 7 nm in every case. The diameter of the cutting tool in all cases is 5 nm and the value of the rotational speed is equivalent to 5.024×10^{13} rad/s (4.797×10^{14} 1/min). Although the latter speed is quite high, it is a reasonable value regarding the dimensions of the workpiece, the feed and the final time of the nano-milling process. As the simulation lasts for several tens of ps, the use of much lower rotational speed would mean that the tool could not have performed a single revolution during the simulation; it would behave almost as a non-rotating rigid tool. Moreover, high rotational speeds have also been reported in nano-milling works in the relevant literature [10,11]. The cutting tool is composed of single-crystal diamond and consists of a number of cutting inserts like a real face milling cutting tool; half of the cases involve a cutting tool with a single cutter and the other cases involve a cutting tool with three identical cutters, each positioned at an angular distance of 120° from the next.

The axis of symmetry of the cutting tool is considered to be aligned with the axis of symmetry of the workpiece in x-axis, as can be seen in Figure 1. The cutters are considered to be rigid and their relative position does not change so that the whole tool behaves as a single body, moving towards the y-axis and rotating around its axis of symmetry at the same time. The total number of atoms in the system are almost 52,000. For the interatomic interactions between Cu and Cu atoms, a suitable EAM potential function is selected, whereas for the interactions between Cu and C, a Morse potential function is selected.
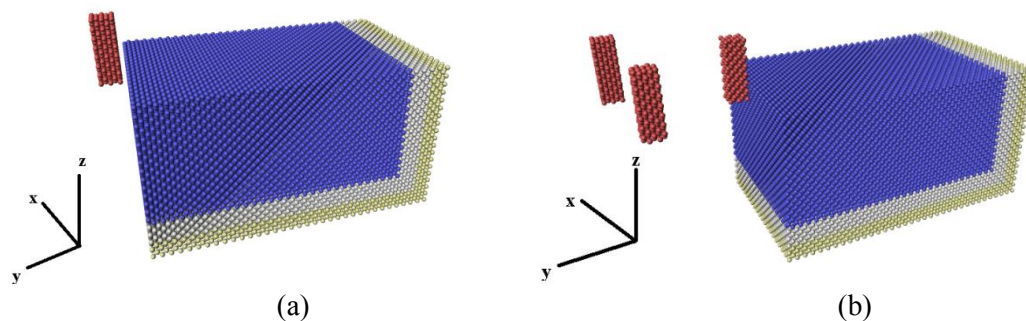

(a)   (b)

Figure 1. Initial configuration of the nano-milling model: (a) for the case with a single cutter, (b) for the case of three cutters.

As can be seen in Figure 1, the workpiece is divided into three different regions of atoms: the atoms in the inner part of the workpiece constitute the Newtonian atoms, which are allowed to move freely when a force is exerted on them by other atoms of the workpiece or the cutting tool, the atoms below the Newtonian atoms constitute the thermostat zone where velocity is rescaled in order to reduce the effect of artificial heat and finally, the boundary atoms which are positioned at the bottom and right side of the workpiece are able to prevent rigid body motion of the workpiece. In order to simulate a workpiece with larger dimensions, periodic boundary conditions are imposed on the yz plane. The cutting tool is initially positioned slightly away from the workpiece and after a short time period the cutter begins to remove material from the workpiece surface. The initial temperature of the workpiece is 293 K and time-step is set to 0.5 fs for all cases. For the simulations, LAMMPS software was employed.

4. Results and discussion

After conducting the aforementioned simulations, the characteristics of nanometric face milling are revealed. In all the examined cases, there are obvious similarities due to the common parameter values employed, such as the depth of cut or the diameter of cutting tool. The various stages of the process resemble the stages of the equivalent macroscopic process. Thus, the cutting tool is beginning to move at a short distance from the workpiece surface and after a while, the cutter comes in contact with the workpiece. As the cutting tool gets closer to the workpiece, the contact of the cutter and the workpiece surface is taking place for a longer period, until the cutter is able to perform material removal for a semi-circle. Due to the fact that the cutting tool diameter is almost equal to the width of the substrate, a large amount of material is removed and so cutting forces are relatively high. In Figures 2a and 2b, two distinct snapshots of nano-milling in the case of a single cutter are presented and in Figures 3a and 3b snapshots for the same time periods for the case of three cutters are presented. As can be seen in these figures, while the cutting tool is moving in the upper surface of the workpiece, atoms are removed and chip is piled in the area in front of the trajectory of the cutter. The differences between cases with higher feed rates or different cutting tool are observable in most cases.
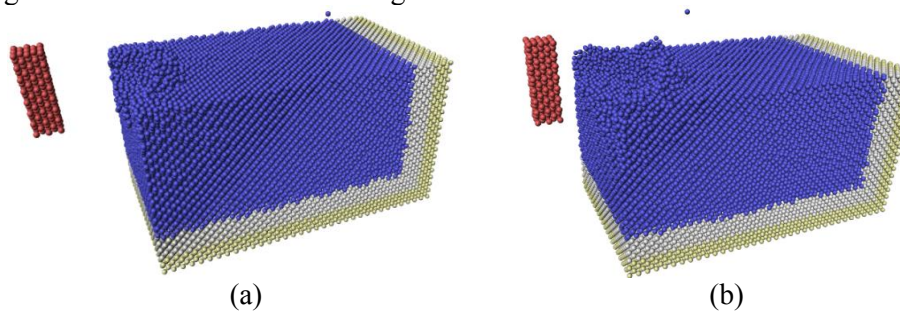

(a)   (b)

Figure 2. Snapshots for a case with a single cutter: (a) at 15 ps, (b) at 25 ps.

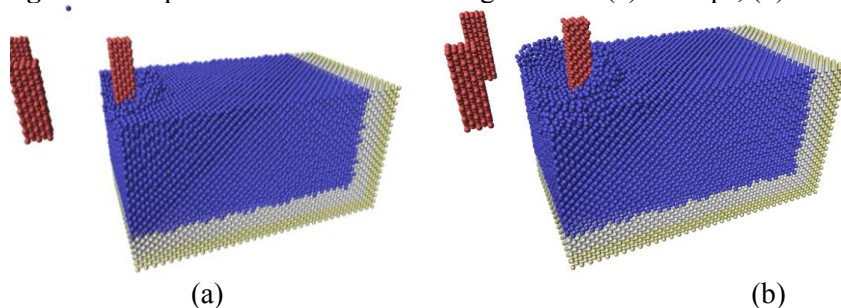(a)   (b)

Figure 3. Snapshots for a case with three cutters: (a) at 15 ps, (b) at 25 ps.

In order to assess more quantitatively the size of the pile of removed atoms in each case, measurements of the height and the length of the pile, in z- and y-directions, respectively, were conducted for the final timestep of each case, i.e. corresponding to 7 nm cutting length. For the cases with the single cutter, the main pile of removed atoms is created in front of the cutting tool. Its height varies slightly, from 21.4 to 22.25 and 24.1 Å, in the cases with feed rate of 100, 200 and 300 m/s, respectively. The length also increases with the feed rate, namely 47.96, 53.94 and 56.7 Å in the three cases. So, it can be seen that, although the same amount of material is to be removed, more atoms are added to the front pile, rather than the sides of the workpiece. However, in cases with three cutters, a different morphology of the pile of removed atoms is observed. In these cases, the height of the pile is smaller and especially in the cases with 200 and 300 m/s the pile in front of the cutting tool is not distinct from the pile of atoms in the sides of the workpiece. Between the last two cases the length is not changed but a slight increase in pile height is observed from 11.13 to 15.42 Å. Thus, it can be seen clearly that the use of a cutting tool with more cutters led to different arrangement of the chip atoms in these cases.

After the observation of process characteristics for the various cases examined in the present work, the analysis of cutting forces for each case was conducted and the components of cutting force in each direction were obtained. As it was anticipated in the case of face milling, the x- and y-component of the cutting force were fluctuating continuously as the relative position of the cutter is continuously changing, leading to variations in cutting forces. When the contact with the workpiece is longer, non-zero values of cutting force are observed for a longer time. The results regarding the time-averaged components of cutting force are presented in Table 1 and also depicted in Figure 4; in this Table, "1-100" denotes a case with 1 cutter and 100 m/s feed rate, "1-200" denotes a case with 1 cutter and 200 m/s feed rate and so on.

Table 1. Results concerning the components of cutting force in each case.

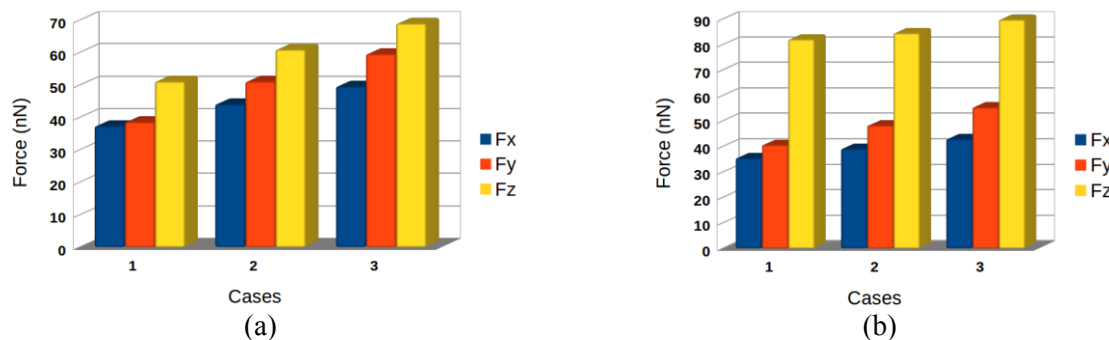| Case	Fx (nN)	Fy (nN)	Fz (nN)
1-100	37.301	38.560	51.054
1-200	44.072	51.010	60.872
1-300	49.510	59.504	68.915
3-100	35.443	40.602	82.043
3-200	39.101	48.283	84.494
3-300	42.957	55.396	89.772

Figure 4. Variation of forces in the case of: (a) cutting tool with a single cutter and (b) with a cutting tool with three cutters.

As can be seen from Table 1, there are clear differences in the time averaged force components between cases with different feed rate, something that is in accordance with findings in the macro-scale, where the feed rate is considered as the most important factor affecting cutting forces, along with the depth of cut. In each case, Fy component is larger than the Fx component and the normal force Fz is larger than all the others. Regarding Fz force, it is observed that is larger in the case of cutting tool with three cutters, due to the more intense contact of the cutting tool with the workpiece in this case. The lower average Fx and Fy values for the cases with three cutters can be attributed to the influence of the feed per tooth to the cutting forces; as feed per tooth values are lower in the cases with larger number of cutters, it is expected that the force should be reduced. Nevertheless, this effect needs to be further investigated in a future study.

5. Conclusions
In the present work, a 3D MD model for nanometric face milling was developed, in order to investigate the characteristics of this process and conduct a preliminary evaluation of the factors

affecting its outcome. Models with a milling cutting tool with one and three cutters are presented for cases with various feed rate values. From these investigations, several conclusions are drawn.

At first, the basic characteristics of nanometric face milling were able to be observed by means of the developed model. It was confirmed that the kinematics of the model were accurate, both in the case of one and three cutters and thus, it can be employed also for more complex and thorough simulations of nano-milling. Regarding chip formation during the process, it was observed that due to the high rotational speed, a few atoms were separated from the workpiece with high speed but the rest of the removed atoms were piled in front of the cutting tool and on the sides of the workpiece. The morphology of the pile of removed atoms was shown to differ considerably between cases with one and three cutters.

Finally, the variations of the components of force were calculated for each case. It was noted that the increase of feed rate resulted in an increase of the cutting forces both for one and three cutters. Especially, for Fx and Fy, it was noted that there is an evident influence of the feed per tooth value to the results as these cutting forces were slightly larger in the case with one cutter because feed per tooth value is greater. The observed trends of cutting force variations are proposed to be further investigated in a future work with a broader range of feed rate, depth of cut and rotational speed values, in order to gain a more comprehensive view of nanometric face milling.

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