Examination of the influence of cutting conditions on nano-metric face milling using MD models

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Abstract. Machining is indispensable in the manufacturing sector for a wide variety of products. In the last years, the field of micro- and nano-scale manufacturing attracted a lot of interest, especially in high-end industries such as the biomedical and electronics industries. In order to improve the efficiency of these processes and understand the various underlying phenomena, it is important to develop relevant theoretical models. However, methods such as the Finite Element Method (FEM), which are well-established in the macro- or micro-scale level are not appropriate for creating models of nano-scale processes, as they treat the materials as continua. For that reason, the Molecular Dynamics (MD) method is usually used for simulations of nano-metric machining processes such as nano-milling. In the present study, a MD model of nano-milling is created and an investigation regarding the effect of cutting conditions such as feed rate and cutting speed on cutting forces, temperature and subsurface damage is conducted.

1. Introduction

Nanotechnology has become increasingly important during the past few decades, as miniaturization of components is essential in various high-end industries such as electronics, biomedical or aerospace industries. In order to be able to fabricate microscopic parts, manufacturing processes have been also extended to micro and nano-scale with the appropriate modifications as it is not directly possible to conduct these processes in the same way as their macroscopic counterparts. With these processes, a higher level of quality and dimensional accuracy can be achieved. Although nano-processing techniques such as lithographic methods and nano-printing are more commonly employed in practical applications, nano-milling is expected to emerge as a possible alternative to these processes [1].

As manufacturing processes are directed to lower scales, several difficulties arise, impeding rapid progress and constraining their capabilities. However, direct experimental work on nano-manufacturing processes is either very difficult to be conducted due to the inability of direct measurements for every quantity or the high cost as well. Therefore, computational methods can be employed to assist in these cases; the requirements of such methods are not satisfied by usual simulation method such as the FEM and thus, atomistic methods such as the MD method are preferred.

Simulations regarding nano-manufacturing process with the use of MD method have been conducted during the past three decades. The first pioneering works were mainly focused on the nano-abrasive processes, especially nano-grinding but also general nano-cutting models were presented. Ikawa et al. [2] studied the minimum chip thickness for given edge radius of a rigid cutting tool and
concluded that minimum chip thickness was mainly affected by the sharpness of the cutting edge. Rentsch and Inasaki [3] developed a MD model for nano-grinding of a copper substrate by a diamond abrasive grain with aim to define the mechanisms of material removal during this process. Maekawa and Itoh [4] studied the effect of friction in nano-machining with a modified Morse potential, as well as tool wear in nano-machining and were able to observe their effect on cutting forces and temperature. Komanduri et al. [5] determined the dislocation motion, subsurface deformation, cutting forces and energy during nano-grinding with an MD model with large negative rake angle tools. Furthermore, models of nano-polishing such as [6] were also developed. Although significant progress was conducted in the case of nano-grinding, however, models of nano-milling have not been developed to a great extent, yet, as can be seen in the relevant literature.

The earliest presented nano-milling model was employed by Cui et al. [7] in a study of nano-groove quality. They employed a two cutting edges rotating cutting tool acting on a copper substrate and compared the results of nano-milling to general nano-cutting. A comparison of the results of nano-end-milling and nano-metric peripheral milling was later conducted [1] and it was concluded that end-milling produced lower cutting forces. Furthermore, end-milling was more stable than peripheral milling, but the latter was able to render grooves of higher quality. Furthermore, a more comprehensive study including the effect of process features, such as the shape of cutting tool and several parameters, namely depth of cut, feed rate and angular speed on cutting forces and the surface quality of produced grooves was also performed by Cui et al. [8]. From this study, it was found that when the depth of cut and feed increase, higher cutting forces are produced and the use of a four cutting edges cutting tool was more preferable than the use of a tool with two cutting edges, as it could lead to a more stable cutting process.

Another work focusing on the parameters affecting the quality of produced grooves was conducted by Cui and Zhang [9], who employed MD models with various cutting tools and milling parameters. The cutting speed as well as groove dimension factors were found to be important concerning the groove quality and it was shown that decreasing of the cutting speed led to better profile quality; the latter was also shown in another relevant work [10]. Furthermore, a similar MD model was applied to other substrate materials, such as nickel and iron [11]. Apart from the end-milling models with multiple cutting edges, other models have been also proposed for the study of nano-milling. For example, Olufayo et al. [12] proposed a box-shaped cutting tool for the modeling of nano-scale milling of copper workpieces. Moreover, Wu et al. [13] presented a model with a rotating conical cutting tool for nano-milling simulations. Recently, a model regarding face milling with multiple cutting inserts was also presented and an investigation of the effect of feed rate for tools with a single and three cutting inserts was conducted [14].

In the present study, an MD model for nano-metric face milling is developed, in order to investigate the effect of various parameters on the process result. More precisely, cases with various cutting speed and depth of cut values are studied and results pertaining to cutting forces, cutting temperature and subsurface damage are presented and discussed in order to determine the importance of each process parameter as well as their recommended values for efficient material removal.

2. MD method

Molecular Dynamics is a computational method, particularly suitable for simulating nano-scale systems. Originally it was employed in the mid-20th century for material science simulations but it was later introduced to other scientific fields as well. In the case of nano-manufacturing, it was first employed almost three decades ago and since then, it has gained more popularity. The importance of MD as a simulation method in nano-manufacturing is related to discrete nature of matter in this scale, which cannot be treated by FEM. An MD model of nano-machining consists of an atomistic scale workpiece and a cutting tool. There does not exist a computational mesh but the components of the system are represented by their exact atomistic structure. The motion of these atoms is calculated according to the application of Newton’s 2nd law on the interatomic forces. The interatomic forces are computed by means of an appropriate potential function, taking into consideration the type of material
e.g. metallic or ceramic and its properties. Especially for metals, the Embedded Atom Model (EAM) potential function is the most suitable although in the past simpler potentials such as the Morse potential were used. After the interatomic forces are computed, the solution of newtonian equations is conducted in order to calculate atomistic trajectories and subsequently in the post processing stage cutting forces, temperature, strain and stress as well subsurface damage can be determined and analysed.

3. Methodology
In the present study, cases of nano-milling under various process conditions on substrates of single crystal copper (fcc) with a rotating cutting tool are carried out with the MD method. More specifically, the depth of cut values are 0.5\(a\) and 1.5\(a\), with \(a\) representing the lattice parameter of the substrate material; feed rate value is 200 m/s and rotational speed is 1.256, 2.512 and 5.024x10\(^{11}\) rad/s. Although the cutting speed value is considered rather high, it is assumed to be reasonable value due to the spatial scale of the system and relative to the feed value and the total cutting length. These values are similar to those reported in the relevant literature for cases of nano-end-milling simulations [8]. As the simulation is carried out up to several tens of ps, it is intended to allow the rotating tool to perform several full revolutions during the simulation time; otherwise the cutting tool would behave like the non-rotating rigid tools. The cutting tool has a diameter of 5 nm and contains three milling cutters; moreover, it is composed of single-crystal diamond.

In any case, the axis of symmetry of the face milling tool is aligned with the axis of symmetry of the workpiece in the \(x\) axis. The cutters are considered as rigid bodies and with a fixed position relative to each other as they belong to the same cutter and rotate at a common rotational speed. Thus, their relative position does not change during the simulation and the whole cutter is moving with the prescribed feed rate towards the workpiece in the \(y\) axis. In the atomistic system, a total of about 59,600 atoms are employed. The interaction between workpiece atoms is modeled by a suitable EAM potential function for Cu-Cu interactions and the tool - workpiece atoms interaction is modeled by a Morse potential function for Cu-C interactions.

![Figure 1. Initial setup of the MD model employed in the present work.](image-url)
the workpiece and, after it engages the workpiece, removes atoms from its surface. The initial temperature of the workpiece is set at 293K and the time-step is 0.5 fs for all cases. For the cases described in the paper, open source code LAMMPS was employed.

4. Results and discussion
At first, after the simulations are carried out, the basic characteristics of the nano-milling process can be directly observed. The cutting tool advances towards the workpiece with the prescribed feed while it rotates and when it engages the workpiece, material is removed. As the cutting tool travels a longer distance in the workpiece, the engagement of cutters and workpiece increases until each cutter can remove material in a semi-circular trajectory, given that the diameter of the cutting tool is smaller than the workpiece width.

From the obtained results, it can be observed that the cutting speed has a direct effect on the deformation of the workpiece atoms and the formation of the new surface. For higher speeds, the material is removed more intensively and quickly a pile of removed atoms is created, as well as an amount of atoms are deposited on the left side of the workpiece due to the counterclockwise rotation of the cutting tool. If the cutting speed was increased, some atoms can even be ejected from the workpiece due to their high speed, whereas for lower cutting speeds at the same feed rate, material is removed more gently as the engagement of cutting tool and workpiece atoms is conducted with less momentum. These can be noted from figure 2(a) and figure 2(b), where two snapshots for the same depth of cut at different cutting speeds are presented.

![Figure 2](image)

**Figure 2.** Selected snapshots of nano-milling at 17.5 ps: (a) at 0.5\(\mu\)m depth of cut and 2.512x10^{11} rad/s rotational speed and (b) at 0.5\(\mu\)m depth of cut and 5.024x10^{11} rad/s rotational speed.

Apart from the observation of the deformation of the workpiece, the investigation of the effects of cutting speed and depth of cut in nano-milling is conducted in terms of cutting forces, temperature and subsurface damage. The time-averaged values of resultant cutting force are presented in Table 1. It can be seen that, as it was anticipated, the resultant cutting force is increasing with increasing depth of cut but also with increasing cutting speed. This is attributed to the fact that the cutters are engaged more intensively with the workpiece atoms, by removing them at a larger velocity and thus, a higher force is developed. Within the range of process parameters employed, the depth of cut seems to play a more important role regarding the resultant cutting force, as a three-fold increase of depth resulted in 1.27 to 1.56 times higher force, whereas a four-fold increase of cutting speed resulted up to 1.27 times higher force.

At the same time, similar trends can be generally observed regarding the process temperature. In this case, the increase of both cutting speed and depth of cut result in higher process temperature, as anticipated. Furthermore, it is interesting that the increase of temperature between cases with rotational speed from 2.512 to 5.024x10^{11}rad/s is considerably higher than the increase of temperature
between cases with 1.256 to 2.512x10^{11} \text{ rad/s}. Although the cutting speed was less important regarding cutting forces, however, it is noted that cutting speed plays a more important role regarding temperature; a three-fold increase of depth of cut results in an increase of temperature up to 1.25 times whereas a four-fold increase of cutting speed consequences to an increase of temperature up to 1.82 times. Thus, its importance is almost similar to the importance of depth of cut.

| Depth of cut | Rotational speed (\text{rad/s}) | Resultant force (\text{nN}) | Max temperature (\text{K}) |
|-------------|--------------------------------|----------------------------|-----------------------------|
| 0.5a        | 1.256x10^{11}                  | 8.3389                     | 366.029                     |
| 0.5a        | 2.512x10^{11}                  | 10.5522                    | 441.002                     |
| 0.5a        | 5.024x10^{11}                  | 10.5989                    | 607.254                     |
| 1.5a        | 1.256x10^{11}                  | 12.9669                    | 403.402                     |
| 1.5a        | 2.512x10^{11}                  | 13.4753                    | 552.126                     |
| 1.5a        | 5.024x10^{11}                  | 13.7835                    | 732.531                     |

In order to analyze the influence of process parameters on the subsurface damage, the study of centrosymmetry parameter (CSP) values is important, as it can reveal variations in the atomistic configuration in the workpiece. The value of CSP for each atom is calculated by the distance of an atom relative to its neighboring atoms in the lattice. According to Tong et al. [15], in a study of fcc copper, the characteristic values of CSP were: CSP<3 for an ideal fcc structure, 3<CSP<5 for a partial dislocation, 5<CSP<8 for a stacking fault, 8<CSP<21.5 for surface atoms and CSP>21.5 for surface edge atoms. The same analysis is conducted in the present work and the results are summarized in Table 2.

| Depth of cut | Rotational speed (\text{rad/s}) | Ideal fcc structure | Partial dislocation | Stacking fault | Surface atoms | Surface edge atoms |
|-------------|---------------------------------|---------------------|---------------------|---------------|---------------|-------------------|
| 0.5a        | 1.256x10^{11}                   | 37678               | 134                 | 291           | 2,028         | 189               |
| 0.5a        | 2.512x10^{11}                   | 37305               | 283                 | 420           | 2,092         | 220               |
| 0.5a        | 5.024x10^{11}                   | 35739               | 1,022               | 958           | 2,356         | 245               |
| 1.5a        | 1.256x10^{11}                   | 37106               | 267                 | 525           | 2,182         | 240               |
| 1.5a        | 2.512x10^{11}                   | 36040               | 658                 | 912           | 2,425         | 285               |
| 1.5a        | 5.024x10^{11}                   | 32650               | 1,735               | 2,129         | 3,473         | 333               |

At first, it is observed that because depth of cut values are low and a small fragment of material is removed from the workpiece, the majority of Newtonian atoms remains undisturbed in the fcc lattice. Moreover, it can be seen that there is clear difference between the various cases and that increased values of cutting speed and depth of cut lead to more deformation of the workpiece, as an amount of atoms are disordered from the ideal fcc structure. More specifically, a considerable increase of atoms pertinent to the partial dislocation or stacking fault categories is attested for high cutting speed. Thus, it can be deduced that in the case of workpiece deformation, it seems that the cutting speed plays a predominant role and a less deformed structure can be achieved by restricting the cutting speed to a suitable limit.

As it was seen by analyzing the results regarding cutting forces, temperatures and subsurface damage, both process parameters are critical for the result of the process, with depth of cut affecting primarily cutting forces and temperature and cutting speed affecting primarily the subsurface damage. Thus, it can be suggested that for the specific feed rate value, the preferred rotational speed for both depths of cut should lie around 2.512x10^{11} \text{ rad/s} in order to achieve material removal with acceptable cutting forces and temperatures value and moderate levels of deformation.
5. Conclusions

In the present study, an atomistic face milling model was presented and introduced to copper nano-milling at different values of cutting speed and depth of cut. From the analysis of the results, various conclusions can be drawn. At first, it was shown that excessive cutting speed can lead to the ejection of atoms from the workpiece surface due to the high velocity that they develop when they engage with the cutting tool atoms; thus there exists a certain limit for acceptable cutting speeds during nano-milling.

Furthermore, analysis of cutting forces, temperatures and deformation revealed that both depth of cut and cutting speed are important process parameters, as depth of cut mainly influences the cutting forces and temperatures, whereas cutting speed was shown to affect considerably the deformation of the workpiece, especially over a certain value. Thus, it was suggested that for every depth of cut, it is preferable to maintain a moderate cutting speed in order to achieve both efficient material removal and less disturbance to the workpiece structure.

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