Molecular dynamics simulation of multi-pass nano-grinding process

Nikolaos E. Karkalos and *Angelos* P. Markopoulos*

National Technical University of Athens, School of Mechanical Engineering, Section of Manufacturing Technology, Heroon Polytechniou 9, 15780, Athens, Greece

Abstract. Grinding involves the use of a large number of micrometric abrasive grains in order to remove material from workpiece surface efficiently and finally render a high quality surface. More specifically, grinding in the nano-metric level serves for attaining nano-level surface quality by removing several layers of atoms from the workpiece surface. The abrasive grains act as individual cutting tools, performing primarily material removal but also induce alterations in the subsurface regions. In order to study the nano-grinding process, Molecular Dynamics (MD) method is particularly capable to provide comprehensive observations of the process and its outcome. In this study, MD simulations of multi-pass grinding for copper substrates, using two abrasive grains, are performed. After the simulations are carried out, results concerning grinding forces and temperatures are presented and discussed.

1 Introduction

One of the most important categories of manufacturing processes are the abrasive processes, which serve for the removal of material from a workpiece, by using numerous abrasive grains. More specifically, grinding can be employed in various occasions for industrial purposes such as the removal of large amounts of bulk material or improving considerably the surface quality of products [1, 2]. The efficiency during material removal and the improvement of surface quality is crucial for the increase of product life and their compatibility in relation to other parts, something that is particularly useful in electronics and biomedical implants industries [3-7].

One of the current trends, in several high-end industries, is the miniaturization of parts. Thus, the study of manufacturing processes in the nano-scale has become a subject of high interest. As the experimental study of such processes and direct measurement of physical quantities is either considerably difficult or expensive, simulation methods are usually preferred. For macro- and micro-scale processes, the Finite Element Method (FEM) is considered adequate and numerous studies have been carried out using this method. However, it is not applicable in the nano-scale, as a non-continuum method is required to describe properly the material structure and tool-workpiece interactions, when this process takes place at this level. Thus, Molecular Dynamics (MD) method can be employed to simulate the nano-scale manufacturing processes.

* Corresponding author: amark@mail.ntua.gr

Although simulations using MD method in other scientific fields have been reported from the 1950s, the earliest MD models for studying abrasive processes have been presented during the 1990s. One of these pioneering works was conducted by Rentsch and Inasaki in 1994 [8]. They employed a model with a diamond abrasive grain acting on a copper workpiece and were able to conduct an investigation on material removal mechanisms during this process. A model including large negative rake angle tools was employed by Komanduri *et al*. [9] in their work concerning nano-scale grinding process. The results of their work included subsurface alterations in the workpiece such as deformation and the existence of dislocations, as well as cutting forces and energy for cases with various process conditions. Shimizu et al. [10] investigated the effect of grinding speed during nano-grinding process using an MD model. Their findings indicate that there exists a limit, related to wave propagation speed for each material, up to which, increase of grinding speed reduces plastic deformation and grinding energy.

Lin *et al*. [11] conducted MD simulations concerning nano-grinding of silicon with a hemispherical abrasive grain. Their results indicated that cutting force variations can be attributed to dislocations movements in the substrates, as well as plastic deformation. Diamond polishing, another abrasive process was also examined by use of MD method. Agrawal et al. [12] employed a MD model for the study of diamond polishing of silicon substrates by spherical abrasive grains and random geometry asperities. After conducting simulation under various process conditions, several important conclusions, regarding material removal rate, abrasive grain condition and process efficiency were drawn. Zong *et al*. [13] created an MD model for diamond polishing with a single diamond spherical grain and a diamond crystal substrate in order to investigate the phenomenon of material removal rate anisotropy. Using this model, they eventually identified the origins of lattice distortion of the substrate and analysis of RDF and coordination number indicated the dependence of material removal rate on the ratio of sp^2 to sp^3 phases.

An important study was carried out by Eder et al. [14] in order to study the wear of rough surfaces during the nano-polishing process. Their model contained a substrate with randomly generated surface topography with several asperities and randomly oriented abrasive particles of cubic and spherical shape. In another study of the same scientific group [15], the effect of the action of each abrasive grain to the wear of a rough surface, created after nano-grinding, was identified and the stability of abrasive grain in respect to their shape and orientation, acting on various surface topographies, was also investigated. Later, several studies regarding peripheral nano-grinding using abrasive grains, which move in a way that resembles the actual trajectory of grinding wheel grains, were presented, for various numbers of abrasive grains [16-18]. In these studies, the effect of process parameters to the grinding forces and temperature as well as subsurface deformation, was determined.

In the present work, an MD model of peripheral nano-grinding with two diamond abrasive grains is created, extending previously conducted work on the same process [16-18], with a view to study the effect of multiple grinding passes to the outcome of the process. More specifically, cases of nano-grinding of copper substrates at 1, 2 and 3 passes are carried out and afterwards, the results concerning grinding forces and grinding temperature are compared.

2 Methodology

In the present work, cases of nano-grinding of 3D copper, namely of Face Centred Cubic (FCC) structure, substrates are considered, completed in 1, 2 or 3 passes. The final depth of cut in all cases is 1.8 nm and the cutting length is 10.12 nm. The abrasive grains consist of single crystal diamond and have the same cubic geometry. The total number of atoms in the

system is about 54,000. For the interactions between copper atoms, the Embedded Atom Model (EAM) potential function is selected [19], whereas the interactions between the workpiece atoms and the carbon atoms of the tool is modelled using Morse potential function, with the required parameters selected from the relevant literature [20]. The atomistic system is depicted in Figure1. In this figure, the two abrasive grains are represented with red colour, the Newtonian atoms in blue, the thermostat atoms in white and boundary atoms in yellow colour.

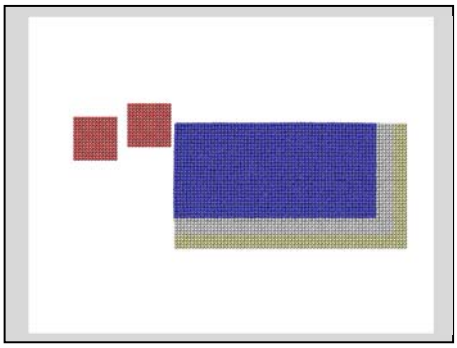


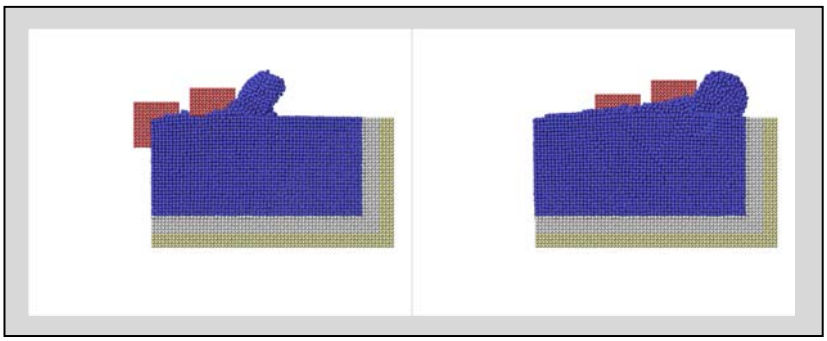
Fig. 1. Schematic of the MD model at the initial timestep.

As it can be seen in Figure1, the abrasive grains are positioned in a single row and the second one has a lower protrusion height; thus, this grain is also able to remove material from the workpiece as it follows the first grain. In all simulations, the horizontal axis is y-axis, the vertical axis is z-axis and the x-axis direction is normal to the yz plane. Both abrasive grains are considered rigid and their velocity is defined in a way which resembles the actual movement of grains of a grinding wheel. The magnitude of grinding velocity is 200 m/s in any case. In the cases where multiple passes are performed, the abrasive grains are returned to their initial position in the y axis with larger velocity than the actual, as no cutting is performed. Then, they are moved towards their new initial position and perform the next grinding pass, at the proper depth of cut. Each pass is performed at equal depth of cut values e.g. in the case of 3 passes the depth of cut for each pass is the 1/3 of the depth of cut in the case of 1 pass. The initial temperature of the substrate is set to 293 K and numerical time-step is 0.5 fs. For the simulations, LAMMPS MD software was employed.

3 Results and discussion

After the simulations were performed, observations on the results for various stages of the nano-grinding process can be conducted. For all cases, at the earliest stages of nano-grinding, the first abrasive grain is approaching the workpiece from a short distance and it starts to interact with it, removing material and creating the chip. As the displacement of the abrasive grain is increasing, a groove begins to form and atoms are displaced either in front of the grain or over the groove walls. After specific time has passed, the second grain is entering the workpiece, removing some material and moves into the previously generated groove by the first grain. The nano-grinding process carries on with the grains moving at the predefined path until the first reaches the boundary of the workpiece. In the case of multiple passes, the abrasive grains are travelling at their initial y-axis position after each pass and then proceed for the next pass at the correct depth of cut. It was observed that at the early stages of the backward movement, the first abrasive grain came briefly in contact with some of the material removed from the second grain and sometimes, the grains interact

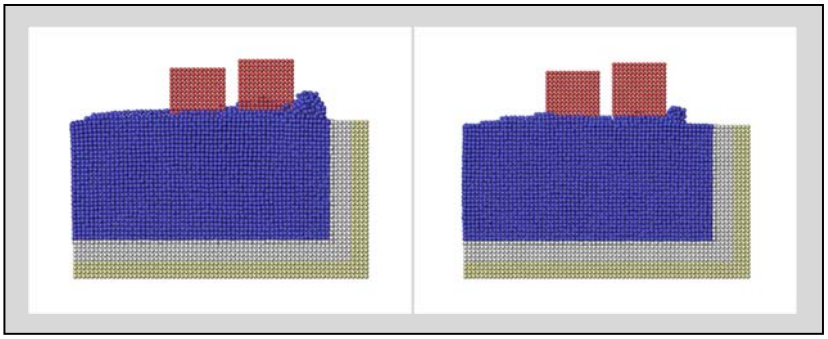
with material from the groove walls, as it is not possible to form exactly straight groove walls. However, force calculation indicates that this interaction is significantly less noticeable than the interaction of grains and workpiece material during the grinding passes.



(a) (b)

Fig. 2. Schematic of the MD model for the case with a single grinding pass at a time-step: (a) in the middle of the process, (b) near the end of the process.

As for the machining chip, in the case of 1 grinding pass as can be seen in Figure 2a and Figure 2b, the interaction between grain and workpiece material produces a chip that continuously increases in height and volume but, when the first grain almost passes from the middle of the total cutting length, the chip height does not increase. It exhibits a larger curvature and eventually, the chip atoms move in front of the cutting tool and towards the x direction on both sides. In the case of 2 grinding passes, the chip height begins to increase considerably only after the first grain is near the middle of its total cutting length and has lower height and volume than the chip in the case of 1 grinding pass, as can be seen in Figure 3a. However at the end of the second pass, the newly removed material is added to the previously created pile of atoms so that the final chip volume is almost the same as in the case of 1 grinding pass. The same observations are made in the case of 3 grinding passes where during the first pass, the chip has a much lower height and volume and is barely noticeable over the workpiece surface in the boundary atoms zone, as can be seen in Figure 3b. Eventually, in the end of the nano-grinding process, its volume is comparable to that of the other two cases.



(a) (b)

Fig. 3. Schematic of MD results during the first grinding pass: (a) in the case of 2 grinding passes, (b) in the case of 3 grinding passes.

After the observation of nano-grinding process characteristics, analysis of grinding forces and grinding temperature is conducted with a view to provide a more detailed insight

into the mechanisms of nano-grinding. In Table 1, the values of force components in the horizontal (y) and normal (z) direction are presented for each case. The calculation of average force is performed from the time when the second abrasive grain enters the workpiece. In the case of 1 grinding pass, the force component in y-axis is larger than the F_y force in the case of 2 passes and the case with 3 passes. However, the F_z force (normal component) is larger as the number of passes increases, possibly indicating that slightly more resistance is encountered by the chip atoms, which have already formed a pile from the previous passes. It is also to be noted that the force during individual passes in the case of 2 and 3 grinding passes is lower, as anticipated due to the fact that the depth of cut is ½ and ⅓ of the initial depth of cut, respectively.

Table 1. Grinding force results for every case.

	1 grinding pass		**2 grinding passes**		**3 grinding passes**	
Pass	F_y (nN)	F_z (nN)	F_y (nN)	F_z (nN)	F_y (nN)	F_z (nN)
1	15.1	11.97	7.98	7.67	4.14	3.06
2	-	-	13.82	14.83	8.47	9.85
3	-	-	-	-	12.41	15.85

In the case of the grinding temperature, the average temperature of workpiece atoms becomes larger, as the number of grinding pass increases, as can be seen in Table 2. In the case of 2 grinding passes, the temperature after the 1st pass in lower than the final temperature in the case of 1 pass, as the depth of cut is the half but the subsequent pass is eventually increasing the final temperature in this case. Similar trends are observed also in the case of 3 grinding passes. Between the two passes, no considerable difference is observed, as anticipated. However, due to the fact that a larger velocity for the backward movement of the abrasive grains was chosen in order to reduce the computational cost, the workpiece was not allowed to cool down further and it is expected that the final increase in these cases would be smaller.

Table 2. Results regarding grinding temperature for every case.

	1 grinding pass		**2 grinding passes**		**3 grinding passes**	
	T (K)		T (K)		T (K)	
Pass	Average	Maximum	Average	Maximum	Average	Maximum
1	453.46	550.42	392.39	434.67	331.88	365.93
2	-	-	560.45	610.72	475.11	533.66
3	-	-	-	-	622.07	680.38

4 Conclusions

In this work, nano-grinding simulations on copper substrates by means of MD method were performed in order to investigate the effect of performing the nano-grinding simulation in several passes with lower depth of cut, instead of using a single pass. From the analysis of process outcome, several important conclusions were drawn.

From the nano-grinding simulations the characteristics of this process, when multiple passes are performed, were observed and chip formation mechanism was determined in each case. Furthermore, when grinding the substrate in multiple passes, the F_y force is shown to become lower as the number of passes increases, whereas the F_z force becomes larger. Temperature is also increasing with the number of passes, as the substrate is processed multiple times. Further research is required to investigate the effect of multiple passes under various grinding conditions and finally determine the most favourable conditions for performing nano-grinding in an efficient way.

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