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MOLECULAR DYNAMICS STUDY OF AFM BASED MACHINING PROCESS

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ABSTRACT

Molecular dynamics study has been performed on a three dimensional model to evaluate the machining process on nickel substrate for Nano-Electro-Mechanical System (NEMS) based applications. Some unique macro level properties of Nickel have attracted attention which might be very useful if considered during nano level fabrication especially NEMS based application. Atomic force microscope (AFM) based diamond tool of 4 nm diameter has been used to simulate the whole process varying the cutting depth and effects of cutting depth on deformation, cutting forces, friction coefficient, specific speed and dislocation have been studied. It has been found that, cutting depth has significant relation on different parameters during nanometric machining process. Increasing cutting depth offers more plastic deformations and dislocations induced in the substrate material and consequently result in a rough surface, which satisfies the results obtained by earlier investigations.

Keywords: Molecular Dynamics, Nanomachining, NEMS.

1. INTRODUCTION

After the first approach to investigate the nanometric machining process with copper in late 1980s, several researches have been already performed to explore the insight of machining process in nanocrystalline materials [1-3]. MD simulation has been a reliable technique over the years for its best suited analyzing ability. Komanduri et al. [4-5] has performed MD simulation of the nanometric machining of mono crystalline aluminium to study material deformation, cutting forces, chip formation, exit failure. Also he has performed some methodology like effect of tool geometry on single crystal copper to study the cutting processes [6]. Those works help tremendously to understand the nanometric machining processes. But small models were adopted in most of the cases which can show lot of boundary effects resulting in unreliable results. Also, due to the small models, most of the previous models were based on two dimensional machining process or quasi-three-dimensional (plane strain) machining process. In previous reported works Morse potential is widely used to study the pair wise interaction between metal atoms and to model interatomic force. It is a pair potential considering only two body interactions. So it cannot properly describe the metallic bonds. But many body EAM potential can describe the phenomenon of metals more precisely and that is why it has been adopted for this simulation purpose [7].

Due to advancement of scanning probe microscopy (SPM)techniques, fabrication of Nano-electro-mechanical system (NEMS) has been proposed to fabricated by atomic force microscope (AFM) based nanomachining process [8]. As material property changes with the reduction of its size to nano level, macro level cutting behavior cannot be applied to analyze nano level fabrications. Therefore, not only the theoretical analysis but also the experimental or high performance simulation methodology should be used to study the micro world cutting processes which will provide sufficient knowledge to explore the frictional behavior, elastic -plastic deformation behavior, cutting mechanisms.

During any kind of machining process, friction plays a significant role. Atomic scale friction covered by the area is known as Nanotribology. Nanotribology involves dynamic atomic interactions at the interface of two materials in relative contact. The difference arising between tribology and nanotribology is primarily due to the involvement of atomic forces. So it is not possible to use conventional tribological method to evaluate the characteristics during nanomachining processes. As nanotechnology is on its developing stage, mechanical characterization and tribological behavior demands careful observations and standardization.

In this paper, AFM based 3D model has been used for MD (Molecular Dynamics) simulation and EAM (Embedded Atom Method) potential has been used instead of Morse potential. A velocity of 50m/s has been chosen to carry out the simulation process. Effects of cutting depth on deformation, cutting forces, friction coefficient, specific speed and dislocation have been studied. A constant cutting length of 7.0 nm has been maintained throughout the machining process to put all the results on same length scale and towards a better comparison.

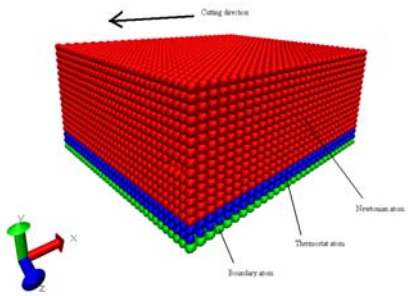


Fig 1. MD simulation model of nanometric machining.

2. SIMULATION METHOD

Fig.1 shows the model for the simulation process. Monocrystalline nickel workpiece has been illustrated out on different zones. Size of the workpiece is 10.56×4.23×8.5 nm and contains 34680 atoms. The lattice constant of Nickel is 0.352nm. An AFM based spherical diamond pin tool has been used as the cutting tool. The cutting process was along negative x-direction, which is taken as the [-100] direction of the FCC lattice of nickel and on (010) surface. Previously, Komanduri at el has been suggested that the (001) [100] combination should be used for performing simulation of machining, if only one orientation has to be used, based on nanometric machining on various cutting directions and crystal orientations[9]. Workpiece consists of three types of atoms- Newtonian atoms, thermostat atoms and boundary atoms. To reduce the size effects, the boundary atoms are kept fixed at their lattice space. Thermostat atoms have been introduced to the system to ensure the heat dissipation which is generated during the machining process [10]. The temperature of the thermostat atom has been kept at 0 K by rescaling the velocities of the thermostat atoms using velocity rescaling method every hundred computational time which corresponds to 0.3 ps. Newtonian atoms obey the Newton's second law of motion. In molecular dynamics, motions of these atoms are determined by the direct integration of the classical Hamiltonian equations of motion using Velocity-Verlet method [11]. A timestep of 3 fs has been used for the velocity Verlet algorithm. Another boundary condition that has been maintained is – periodic boundary condition which has been maintained along the z direction. It provides the means to minimize effects of simulation scale. All models were subjected to relaxation for equilibrium state at zero temperature by energy minimization using the conjugate gradient method to allow the models to reach natural and dynamical equilibrium status consistent with the specified temperature.

The AFM tool used in this simulation has the shape of a sphere and constructed with perfect diamond lattice with a diameter of 4.0 nm. A constant cutting speed of 50 m/s has been used along a cutting distance of 7.0 nm. Cutting depth has been varied from 0.5 nm to 2.0 nm. The initial temperature of the workpiece is 0 K.

The force acting on the system is obtained by calculating the forces acting on the atom by the surrounding atoms and encapsulating them. This calculation has been performed using interatomic potentials. Morse potential is a pair wise potential and not only computationally inexpensive but also simple compared to EAM potential [12].

The EAM method has been originated from the density-function theory and based upon the approximation that the cohesive energy of a metal is governed not only by the pair-wise potential of the nearest neighbor atoms, but also by embedding energy related to the "electron sea " in which the atoms are embedded. This electron density is approximated by the superposition of atomic electron densities. For EAM potential, the total atomic potential energy of a system is expressed as:

$$E_{tot} = 1/2 \sum_{i,j} \phi_{ij}(r_{ij}) + \sum_{i} F_i(\overline{\rho_i}) \qquad (1)$$

Where φ_{ij} is the pair-interaction energy between atoms i and j and F_I is the embedding energy of atom i. ρ_i is the host electron density at site i induced by all other atoms in the system, which is given by:

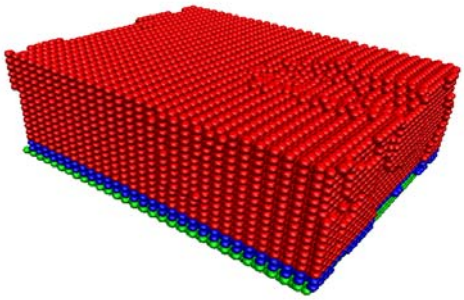
$$\overline{\rho_i} = \sum_{j \neq i} \rho_j(r_{ij}) \qquad (2)$$

There are three different atomic interactions in this simulation of nanometric machining process - the interaction in the workpiece, the interaction between the workpiece atoms and the tool atoms, the interaction in the tool atoms. The EAM potential function for nickel developed by Foiles [13] is used here for the interaction of the substrate atoms. EAM potential has been used instead of pairwise morse potential because the EAM provides a more realistic description of the metallic cohesion, although using morse potential the energetics of an arbitrary arrangements of atom can be calculated quickly, but the ambiguity inherited by the volume dependency is avoided on EAM method. For the Ni-C atoms interaction, morse potential has been adopted as there is no existing EAM potential available to describe the behavior of interactions between Ni-C atoms. It has been adopted from Fang et al. [14] as D=1.0094 eV, α =0.19875 nm $^{-1}$ and r_0 =2.559 nm. The Lorentz-Berthelot mixing rule was used to estimate the interatomic Morse potenitial for Ni-C interactions. For the interactions between the tool atoms, also Morse potential has been adopted where D=2.4230 eV, α=0.25550 nm $^{-1}$ and r_0 =2.522nm. But as stiffness of Diamond tool is much harder than the stiffness of Nickel atoms, the tool can be considered as a rigid body. In this approximation, the interaction force between tool atoms will have no effect on tool atoms. All the simulations of this model use parallel molecular dynamics program LAMMPS [15].

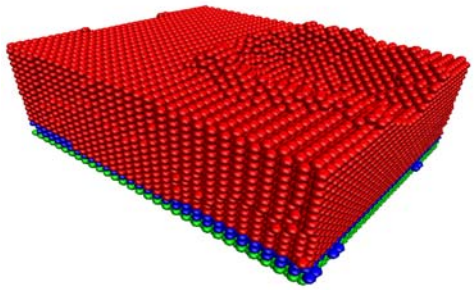
3. RESULTS AND DISCUSSIONS

A three-dimensional model has been used for current study of AFM-based nanometric machining process on monocrystalline nickel using an AFM spherical tool. Cutting depths of 0.5, 1.0, 1.5 and 2.0 have been simulated and their effects on deformation, machining forces, tribological behavior and dislocations have been observed. The atoms have been subjected to relaxation to

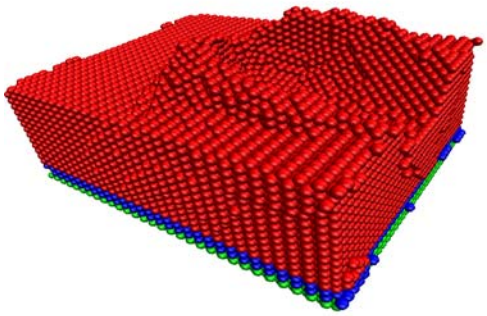
minimize the energy of the system and to allow the system to reach equilibrium condition. It has been done after configuring the workpiece and tool atoms in their perfect lattice structures. The MD simulation code uses LAMMPS, which is an open source code. The discussion provided below is not only from the plots of MD simulations but also from careful observations of the MD simulations. For visualization, an open source molecular visualization program namely VMD- Visual Molecular Dynamics has been used [16].



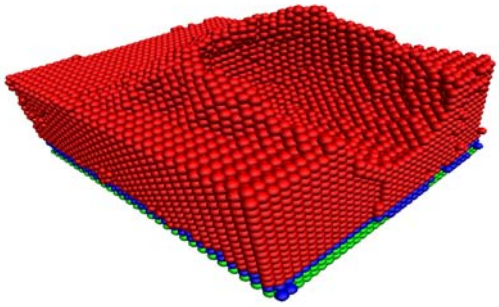
(a) At 0.5 nm



(b) At 1 nm



(c) At 1.5 nm



(d) At 2 nm

Fig 2. Deformation behavior of machining process at different cutting depths of 0.5, 1, 1.5 and 2 nm.

3.1 On the Nature of Deformation

Fig: 2 shows the different states of cutting process during tool travel along the workpiece material with varying cutting depth. The effects have been observed carefully. As it has been known from solid state physics, as a result of attractive and repulsive forces, metallic atoms are not only arranged in a specific pattern but also they maintain an equilibrium distance in their crystal structures. Conducting a cutting process on a crystallographic material structure will generate disturbance throughout the metallic structure. The arrangements of the atoms will be changed to create room for the tool to travel along its surface. Hence the term deformation takes place. As the tool touches the surface, the crystal structure of the workpiece shows adhesion features with the tool atoms. But with the advancement of the tool on its surface, this adhesion feature no longer exists. Rather it turns into repulsive nature and the interatomic bonds between workpiece material breaks due to the advancement of tool atoms. Accumulation of workpiece atoms takes place in front of the tool. In has been found from the simulation that the accumulation not only takes place in front, but also beneath the tool edge and thus chip is formed. Also with the advancement of tool atoms on substrate material surface, atoms pile up on both side of the tool. As tool goes forward, these atoms flow towards their respective piling directions to allow the tool to travel. As cutting depth increases, this accumulation and piling up occurs in greater scale. So deformation occurs in large scale. To allow the workpiece to reach relaxed state, after certain period, atoms in workpiece rearrange in crystal structure. Thus dislocation nucleates and the atoms slip past each other.

3.2 On the Nature of Forces

In the current study, force in the direction parallel to cutting direction has been considered as the Tangential force(x axis) and force in the direction perpendicular to the cutting direction has been considered as Normal force(y axis). The variation of tangential force Fx with cutting distance for the different cutting depth has been plotted in Fig.3. Sudden rise in the forces in the initial stage can be explained as, as the tool atoms and the workpiece atoms pass the adhesion period, repulsion takes place and workpiece material undergoes complex elastic and plastic deformation. After that, it gradually reaches to a steady state. Although for different cutting depths the magnitude is different. The variation is still there in the steady state. More precisely, the variation can be termed as “quaisi-periodic variation.” The same phenomenon has been reported by Buldum and Ciraci et al [2]. That MD simulation was performed using a sharp Ni tip on a Cu substrate. It can be seen from the MD

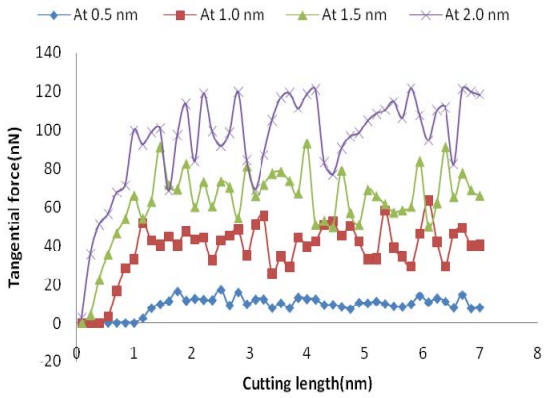


Fig 3. Variation of tangential force for four different cutting depths of 0.5, 1 , 1.5 and 2 nm.

simulation of current study that as the cutting depth is less, the nature of the steady state is more periodic. With the increase of cutting depth, steady state tends to deviate and presence of rapid fluctuations can be identified. And increased cutting depth requires more cutting force for material removal. That can be explained as; more material accumulates in front of the tool as cutting depth increases and more the cutting force is required for the advancement of the tool and material removal. The time averaged cutting forces has been presented in Fig.4 with the variation of cutting depth. It has been considered after reaching the steady state which is from 1.5 to 7.0 nm of travelling distance and sudden fluctuating components has been cut off. Although it has been found that, the natures of the curves are similar only varying in magnitude. Both the tangential force and normal force increases with the increase of cutting depth. But the tangential cutting force increases rapidly comparing to the normal force. The ratio of normal force to tangential force changes from more than 6 to almost 1. It seems that with increase of cutting depth, contribution of forces is more in tangential force rather than in normal force as higher cutting force is required for the larger cutting depth.

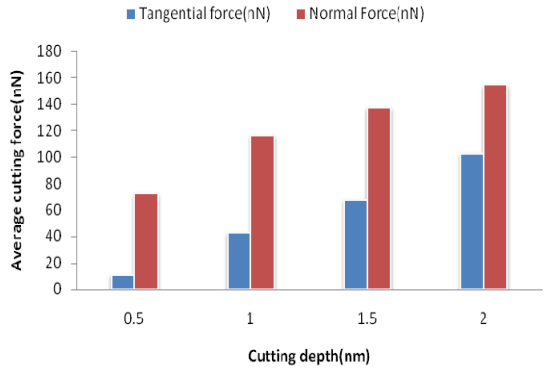


Fig 4. The time averaged cutting forcs for the different cutting depths of 0.5 ,1 , 1.5 and 2 nm.

3.3 On the Nature of Friction

As friction arises from the contact followed by relative movement of two surfaces, it is of obvious need to realize the role of friction in any sort of machining process. And nevertheless, for a sophisticated process like nanomchining it is of immense importance. The values of tangential force and normal force obtained in steady states are listed in Table 1. The friction coefficient is also listed, which is the ratio of tangential force to

Table 1. MD simulation results for varying cutting depths.

Cutting depth(nm)	Tangential force(nN)	Normal force(nN)	Friction coefficient
0.5	10.906	72.455	0.15
1.0	42.597	116.338	0.366
1.5	67.505	137.228	0.492
2.0	102.752	154.573	0.665

normal force. Fig. 7 shows the relation between co-efficient of friction with the variation of cutting depth which has been found to vary from 0.15 to 0.66. Individual cases have not been plotted to save the length of the paper. It has been found that it in individual cases, after reaching the steady state, the friction coefficient is constant but larger in magnitude for larger cutting depth. The co-efficient of friction increases almost linearly with the variation of cutting depth. It can be interpreted as, with the increase of cutting depth, more tangential force is required for tool travel. Because, more material

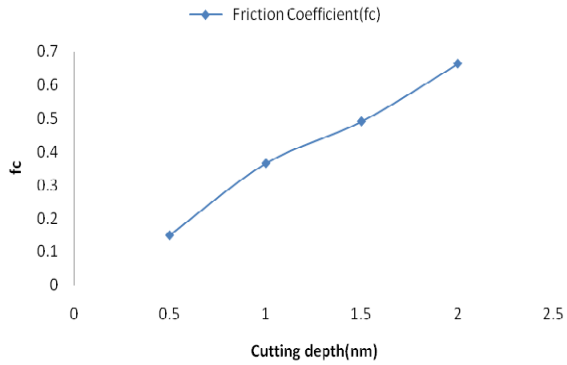


Fig 5. Variation of friction coefficient (fc) with different cutting depths of 0.5, 1 ,1.5 and 2 nm.

accumulates in front of the cutting tool and requires more external force in cutting direction to remove them. As well as the friction coefficient increase. As friction is the measure of the resistance, this can be utilized to understand the resisting behavior during AFM-based machining. The friction coefficient has been found to be more dependent on the tangential force than normal force.

4. CONCLUSIONS

3D molecular dynamics simulation using EAM (Embedded Atom Method) has been carried out on single crystal Nickel using AFM-based nanomachining process for NEMS based application. Possibilities has been evaluated varying the cutting depths (0.5, 1, 1.5 and 2 nm) and observing its effects on forces, deformation behavior, tribological behavior. On the basis of obtained results from the MD simulation, following conclusions can be drawn:

The smaller is the cutting depth, the earlier the cutting force reaches to the steady state. Still the variation exists which can be termed as a "quaisi-periodic" variation [2]. Further study should be carried on to explain this nature and put that into a specific and well-defined function with different cutting parameters. Cutting depth has a major role in nano-machining process, especially in AFM-based machining process. With the increase of cutting depth, machining process is followed by more complex not only elastic deformation but also plastic deformation. The more is the cutting depth, more dislocations generates and nucleates affecting more workpiece material. The frictional coefficient is more dependent on tangential force than the normal force. As with the increase of cutting depth, magnitude of both tangential and normal force increases, but significant contribution goes to tangential force which results in increased frictional coefficient.

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7. NOMENCLATURE

Symbol	Meaning	Unit
Fx	Tangential Force	(nN)
Fy	Normal Force	(nN)
fc	Friction coefficient	---

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